

Project ADMIRE
A Multiscale Framework To Enable
Underground Hydrogen Storage:
Thermodynamics of Storage

Dr. Thejas Hulikal Chakrapani
Prof. Hadi Hajibeygi

27th March, 2023

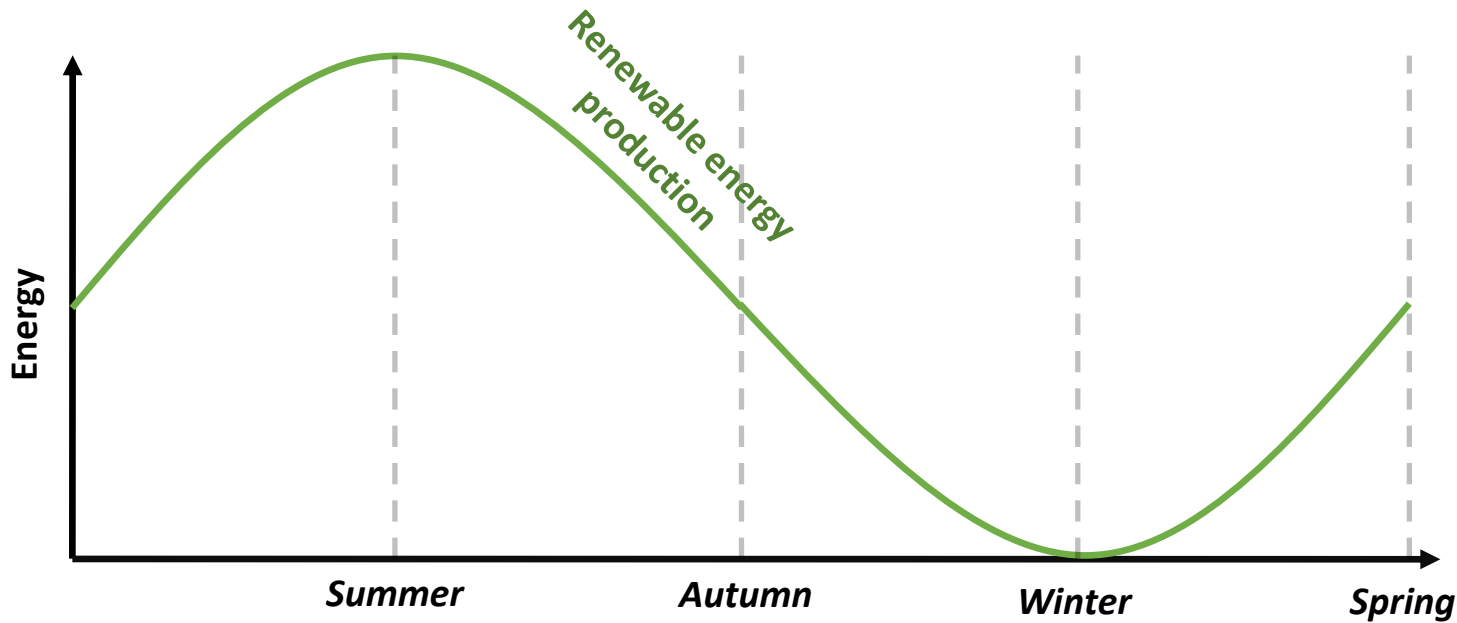


ADMIRE
Hydrogen Lab



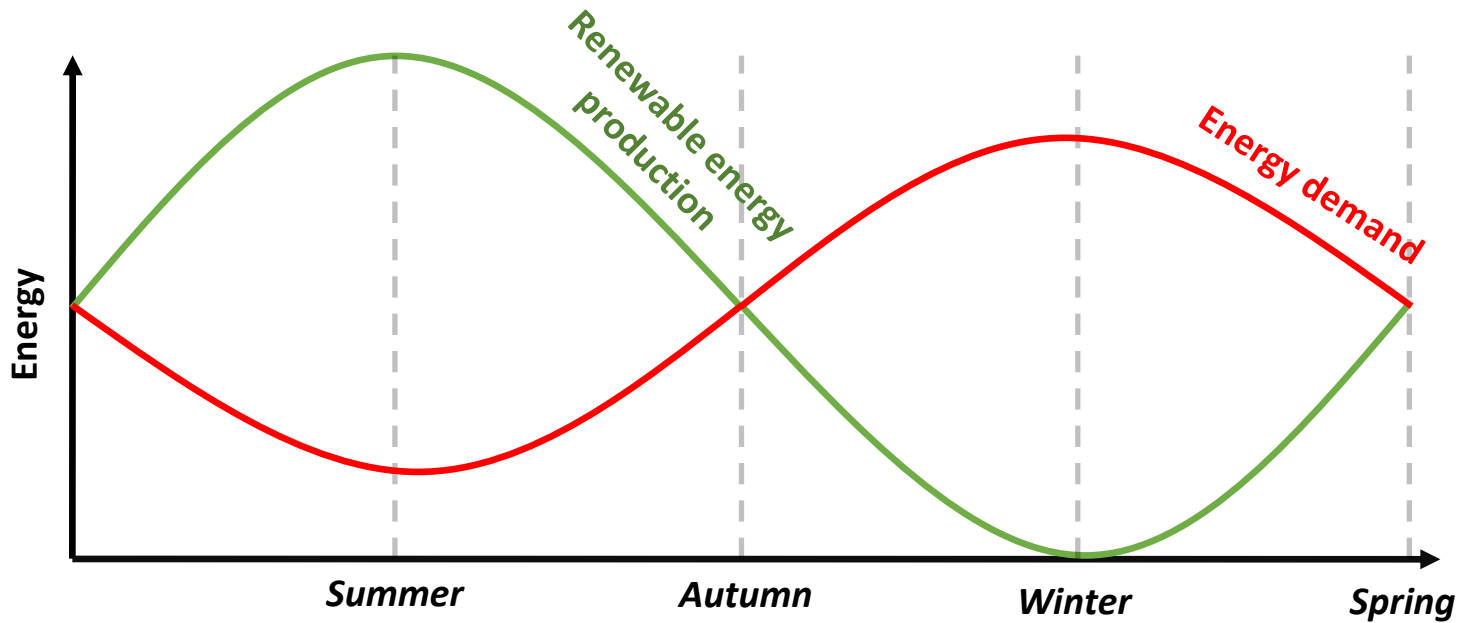
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Why Underground Hydrogen Storage?



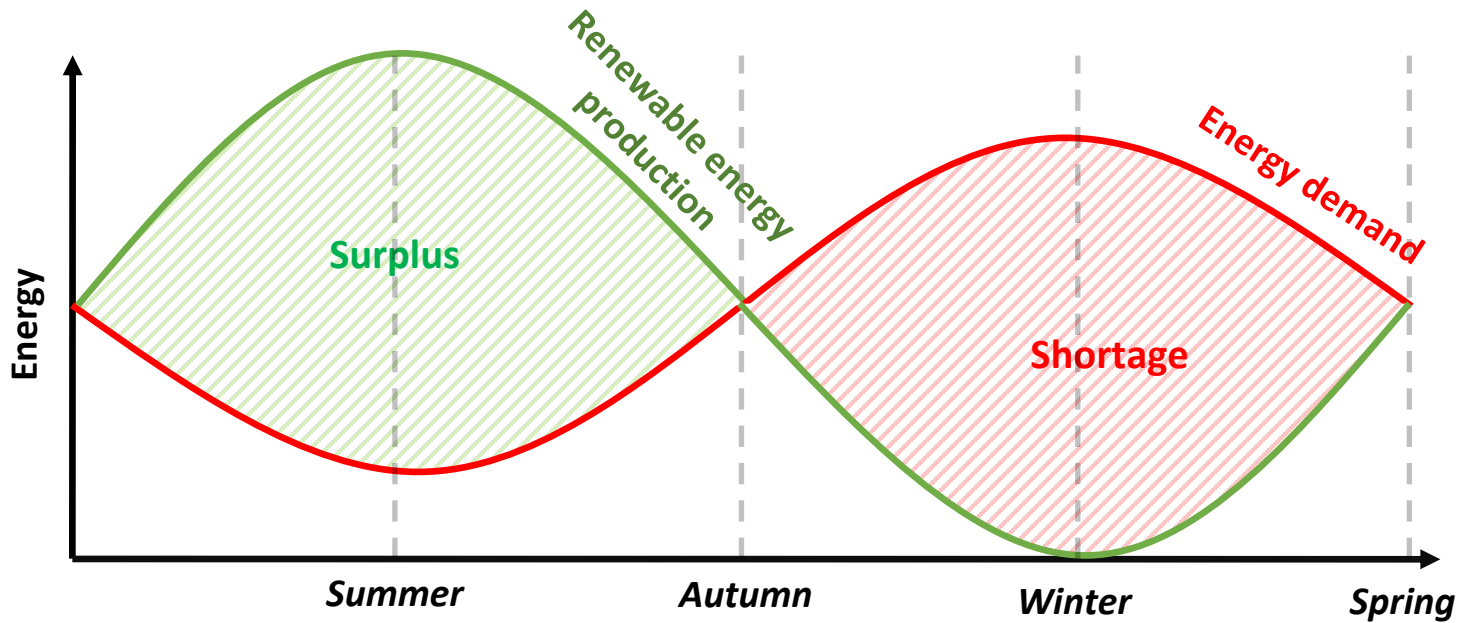
Slides from MSc defence presentation Willemijn van Rooijen

Why Underground Hydrogen Storage?



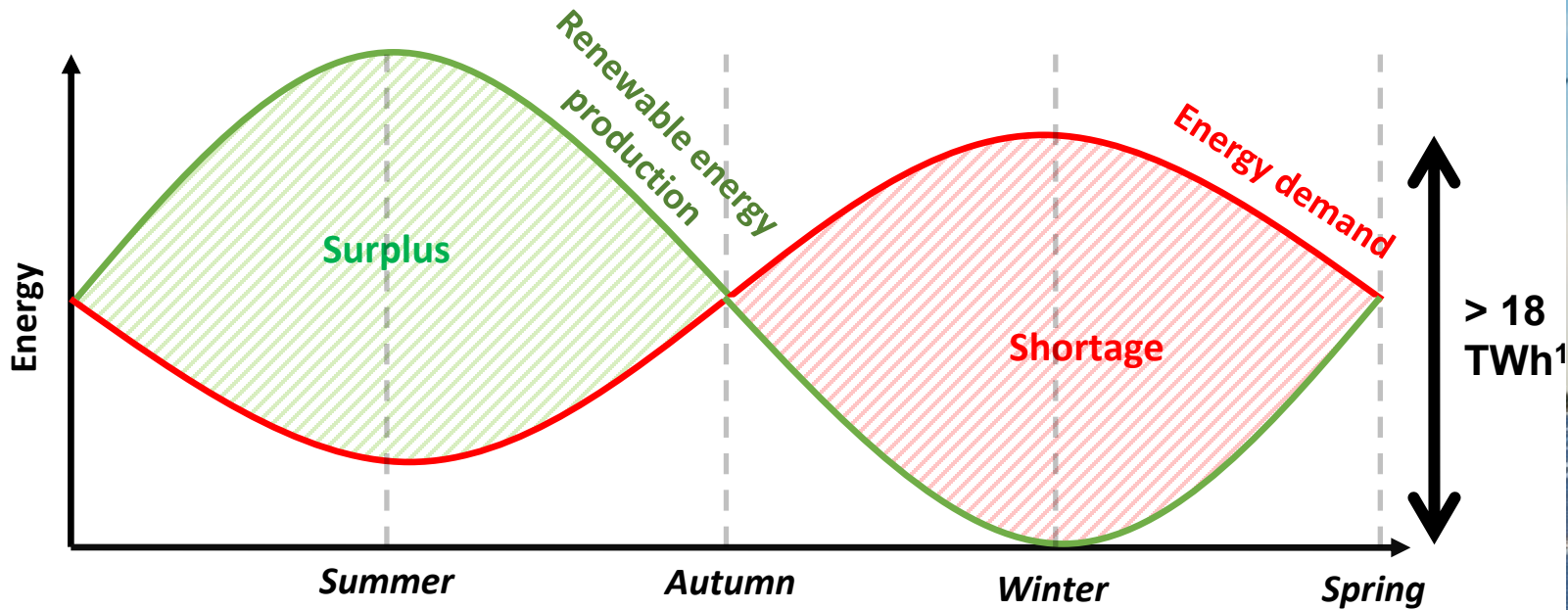
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Why Underground Hydrogen Storage?



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Why Underground Hydrogen Storage?



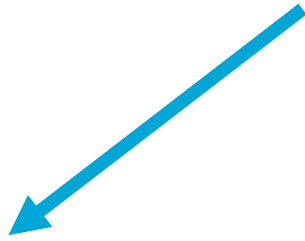
1: Ondergrondse energie opslag in Nederland 2030 – 2050 (EBN & TNO)



Slides from MSc defence presentation Willemijn van Rooijen

Why Underground Hydrogen Storage?

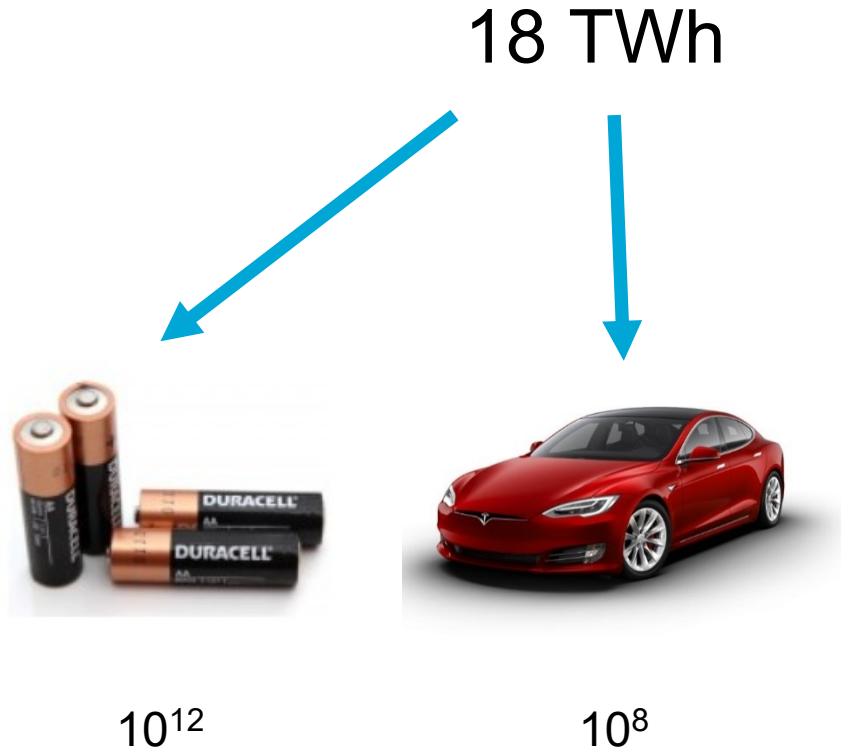
18 TWh



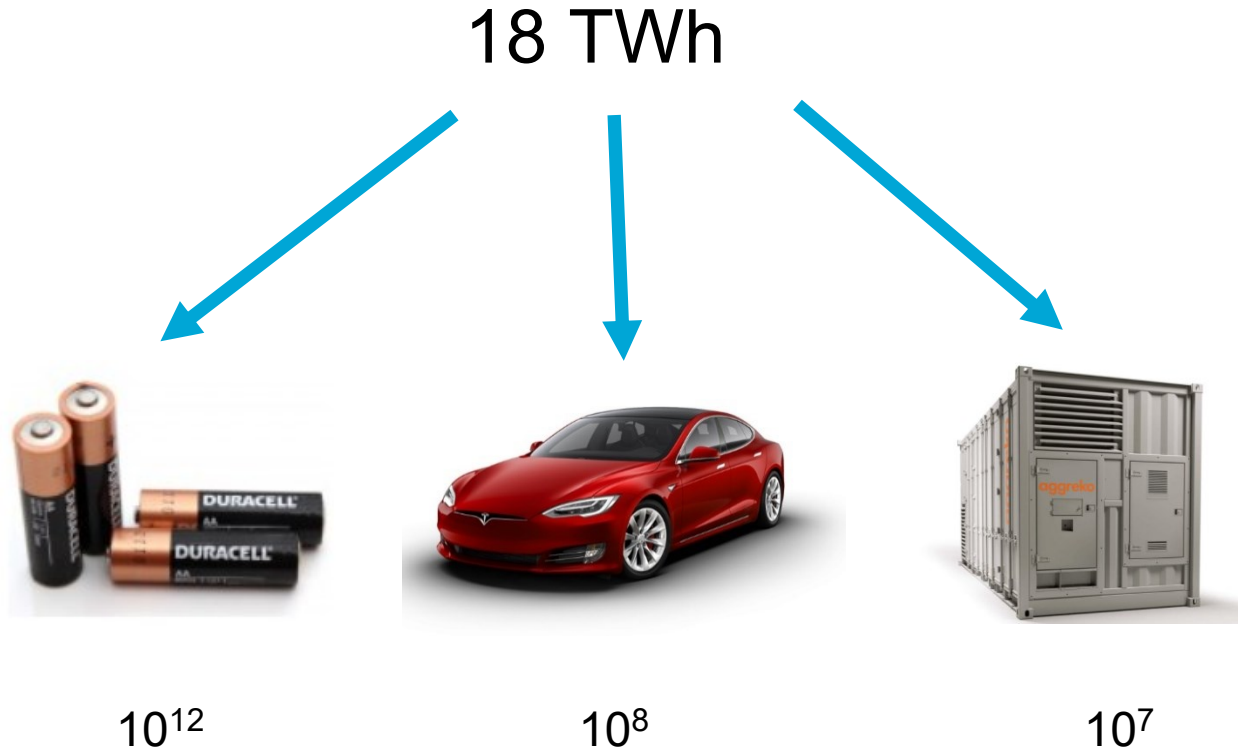
10^{12}



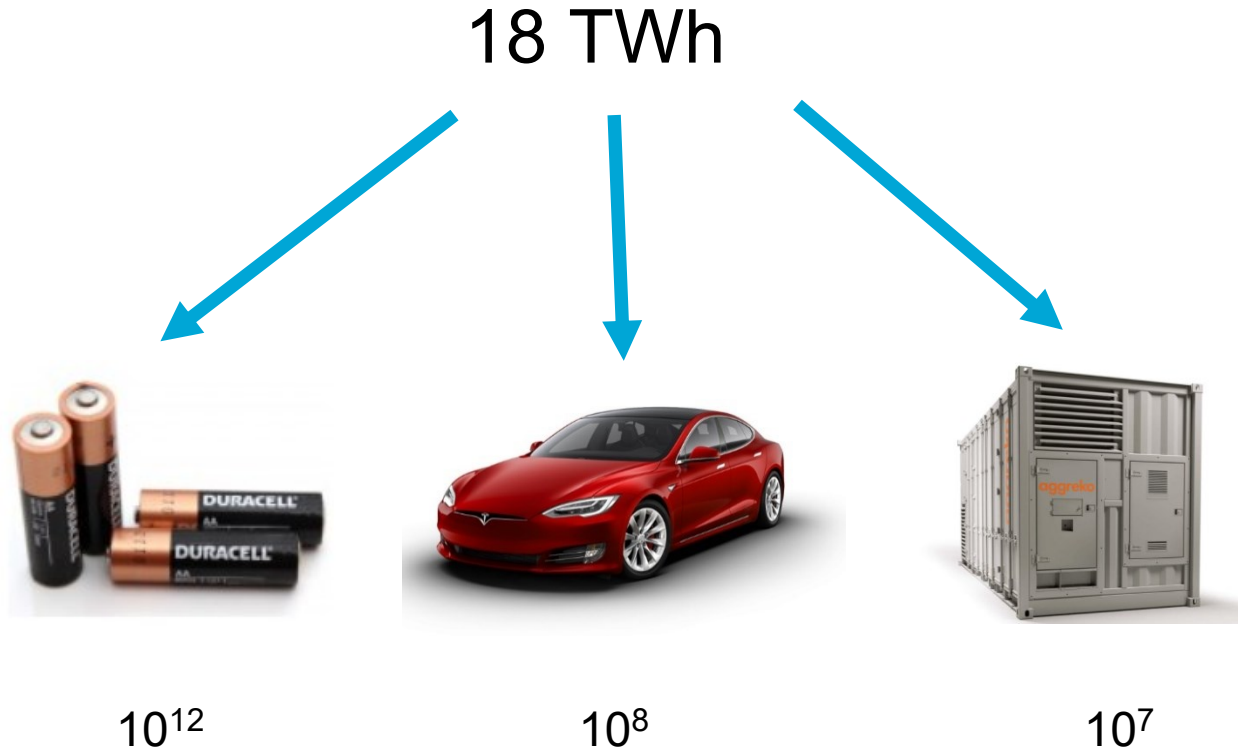
Why Underground Hydrogen Storage?



Why Underground Hydrogen Storage?



Why Underground Hydrogen Storage?



Upscaling of H₂ storage is key for energy transition.

Giant reservoirs allows for TWh storage!



Underground Hydrogen Storage (UHS)

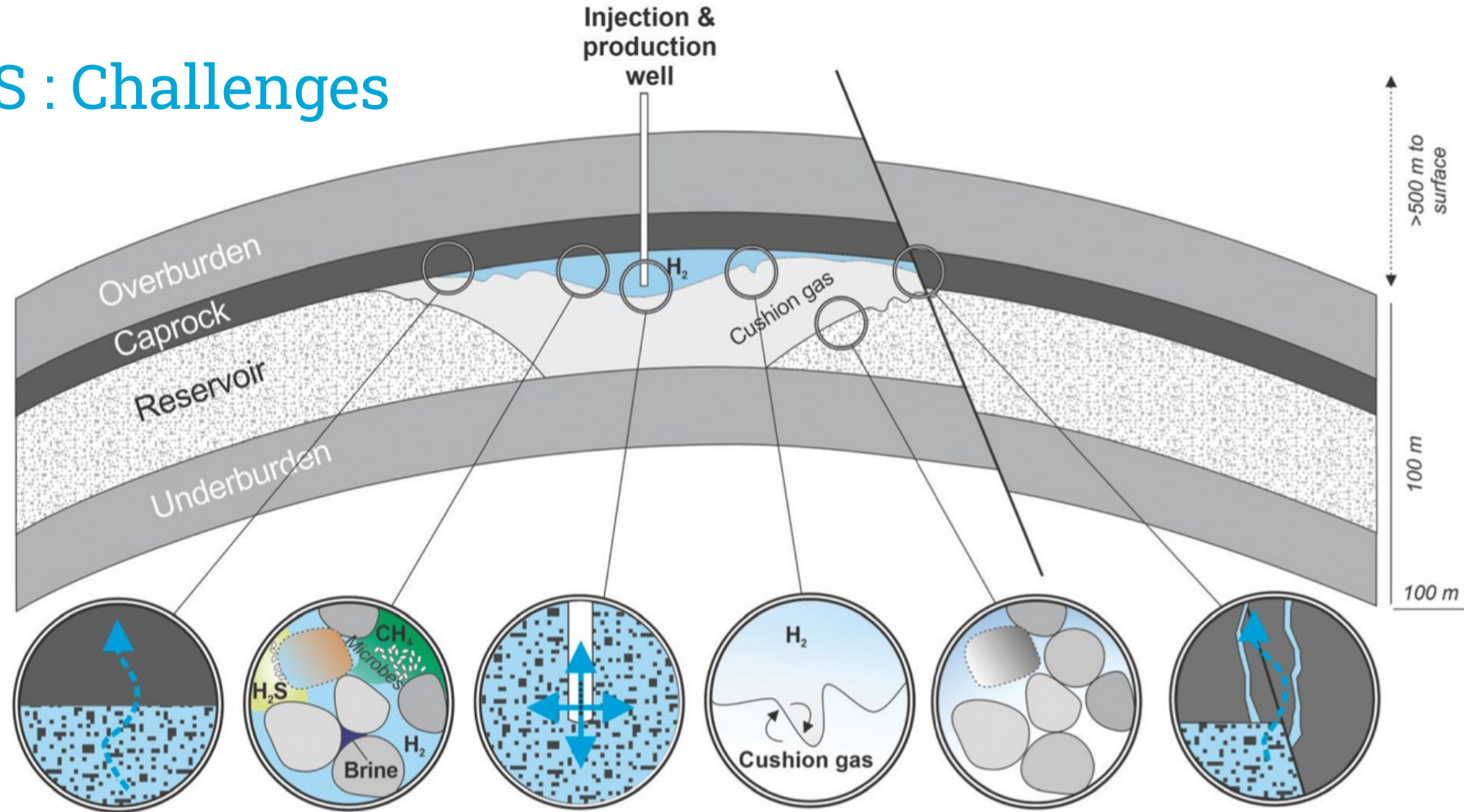


Porous reservoirs



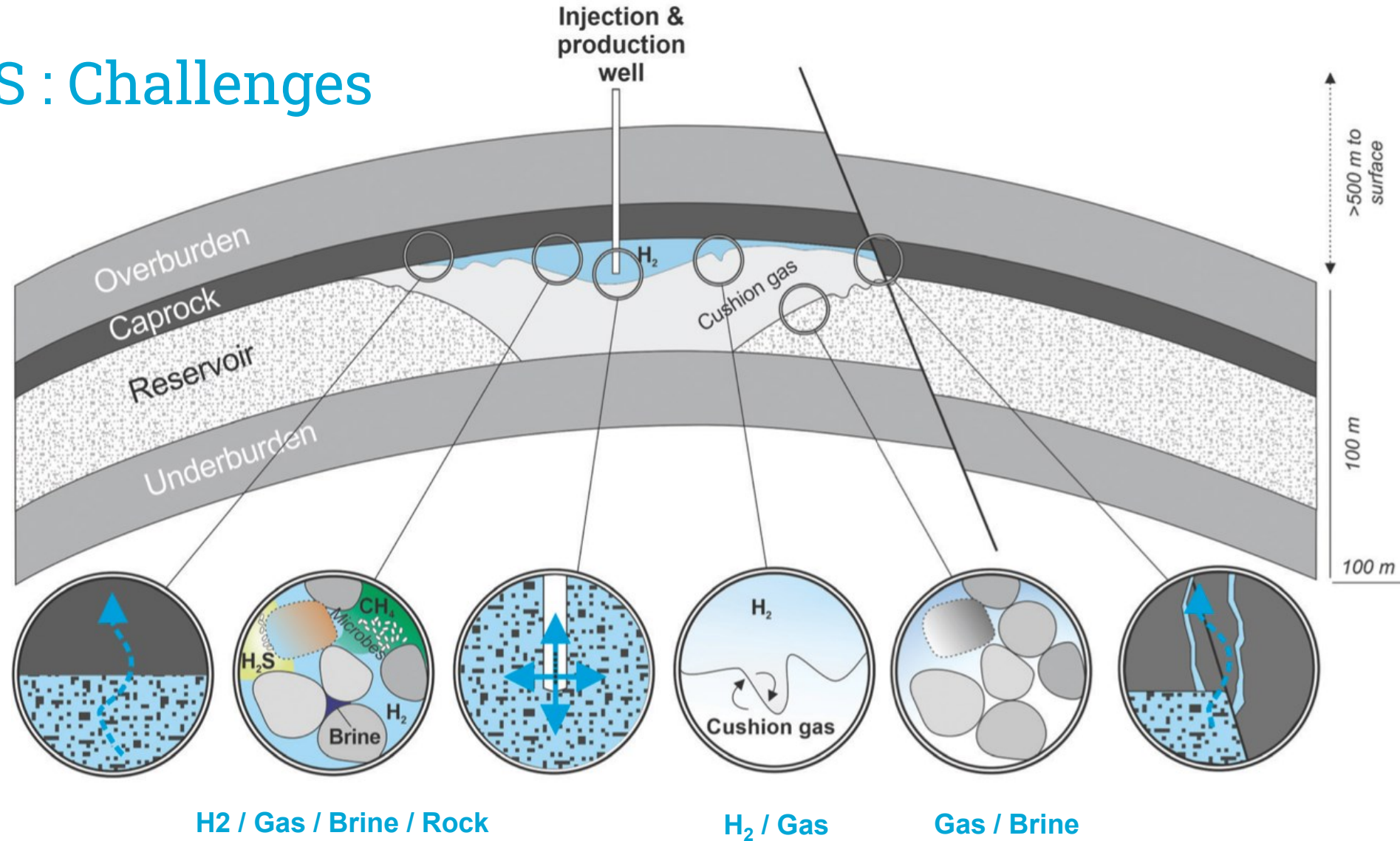
Salt Caverns

Enabling UHS : Challenges



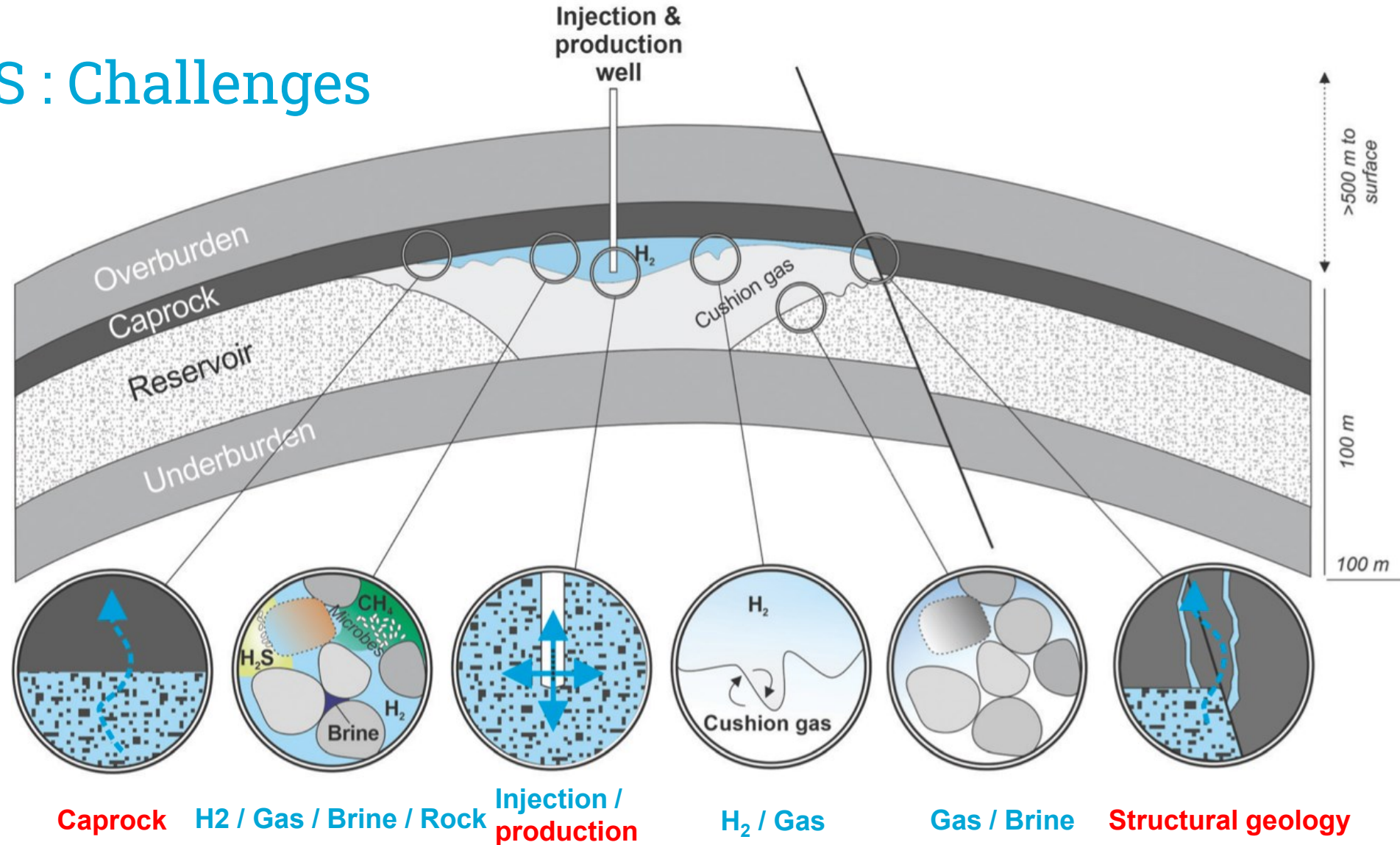
Enabling large-scale hydrogen storage in porous media – the scientific challenges, Heinemann et al., *Energy Environ. Sci.*, 2021, **14**, 853

Enabling UHS : Challenges



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Enabling UHS : Challenges



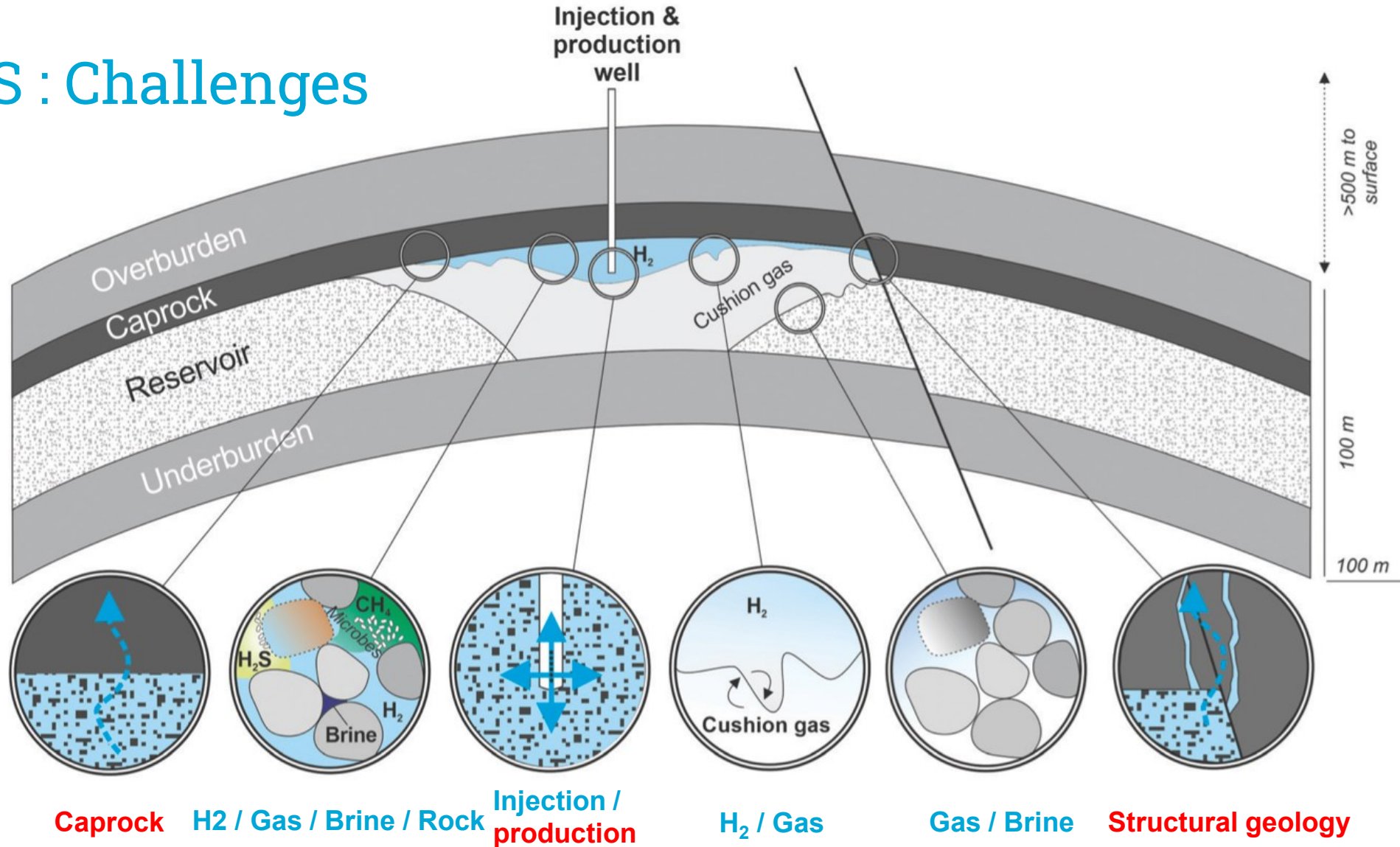
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Enabling UHS : Challenges

Heterogeneous media

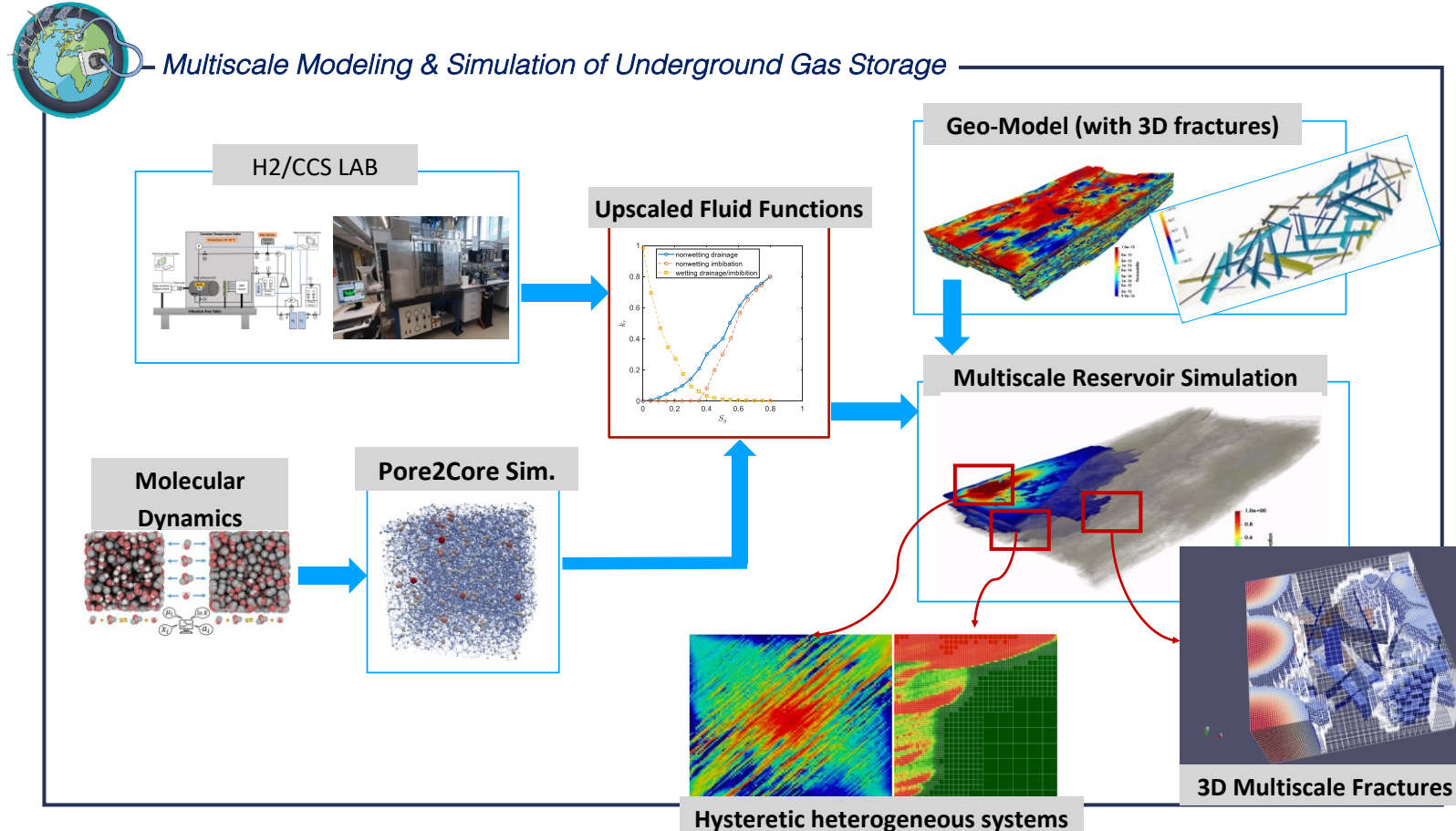
Hydro-Thermo-Mechanics

Multiscale (nm to km)



Enabling large-scale hydrogen storage in porous media – the scientific challenges, Heinemann et al., *Energy Environ. Sci.*, 2021, **14**, 853

Project ADMIRE : A Multiscale Framework



Synergy between experiments, simulations and modelling

Picture from: *Multiscale Modeling Lecture Notes*, Hajibeygi, 2020

Team ADMIRE

Together with many collaborators in
Geosciences, Math, Mechanical
Eng.& Techno-Economics



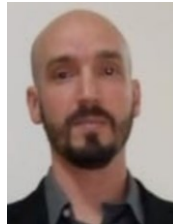
Hadi Hajibeygi



Maartje
Boon



Yuhang
Wang



Herminio
Tasinofo



Thejas
Hulikal
Chakrapani



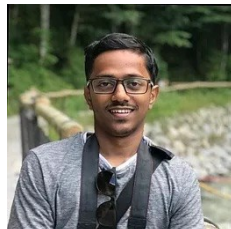
Debanjan
Chandra



Artur
Castiel



Leila
Hashemi



Kishan
Ramesh Kumar



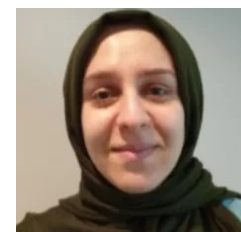
Willemijn
van Rooijen



Mengjie
Zhao



Fangxiang
Xu



Sara
Behbahani



Johnno
van Ijsseldijk



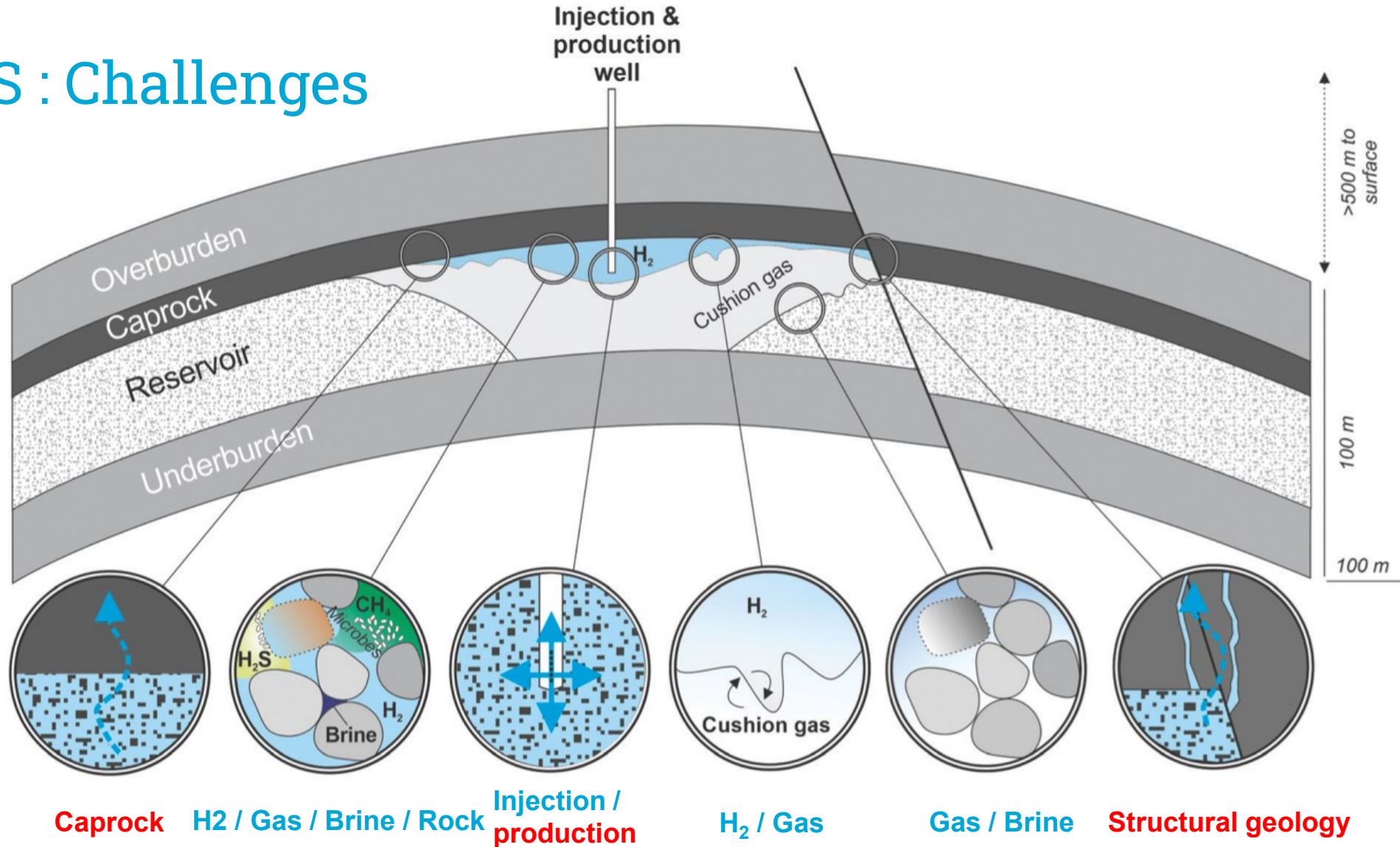
Ziliang
Zhang

Enabling UHS : Challenges

Heterogeneous media

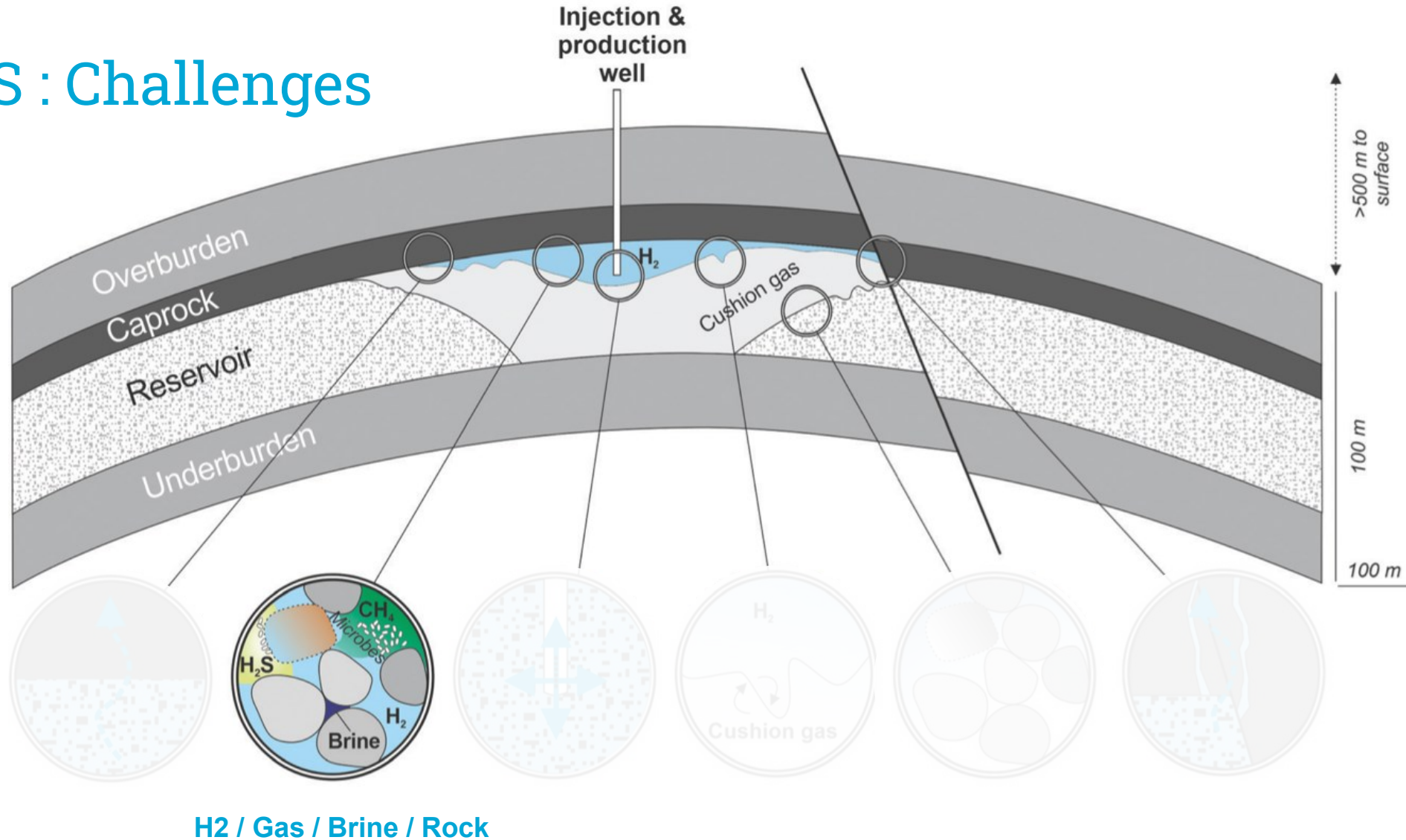
Hydro-Thermo-Mechanics

Multiscale (nm to km)



Enabling large-scale hydrogen storage in porous media – the scientific challenges, Heinemann et al., *Energy Environ. Sci.*, 2021, **14**, 853

Enabling UHS : Challenges



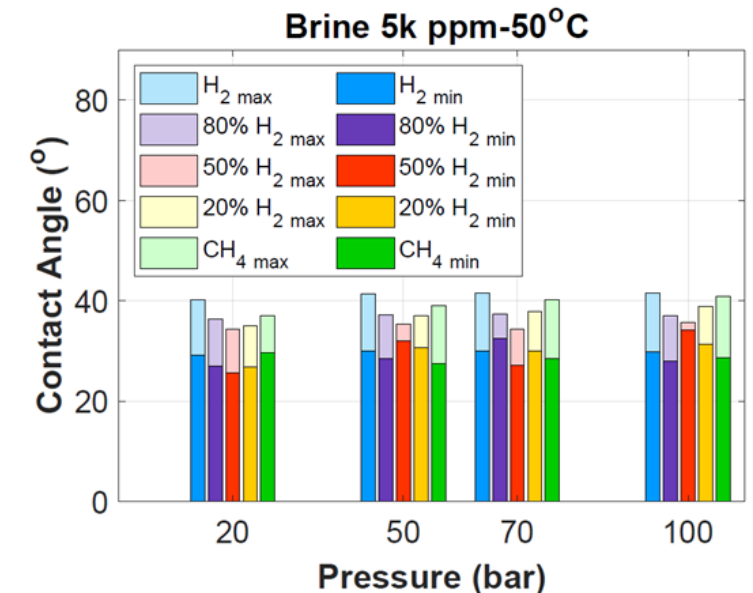
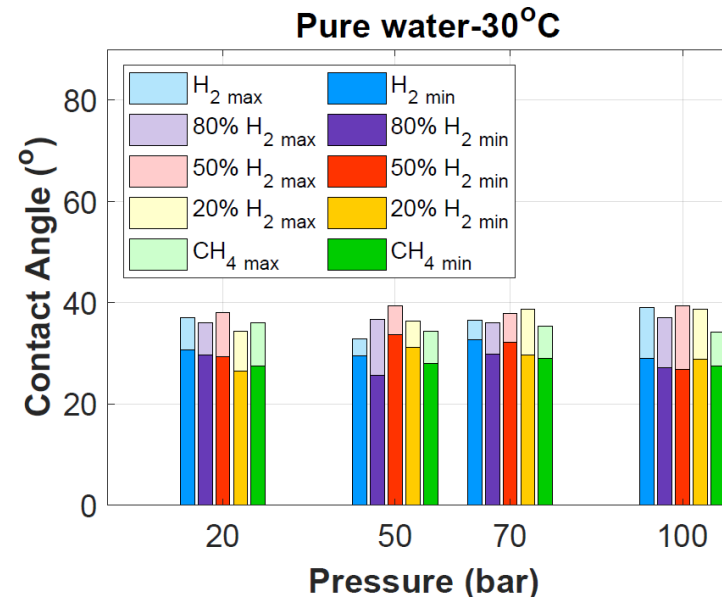
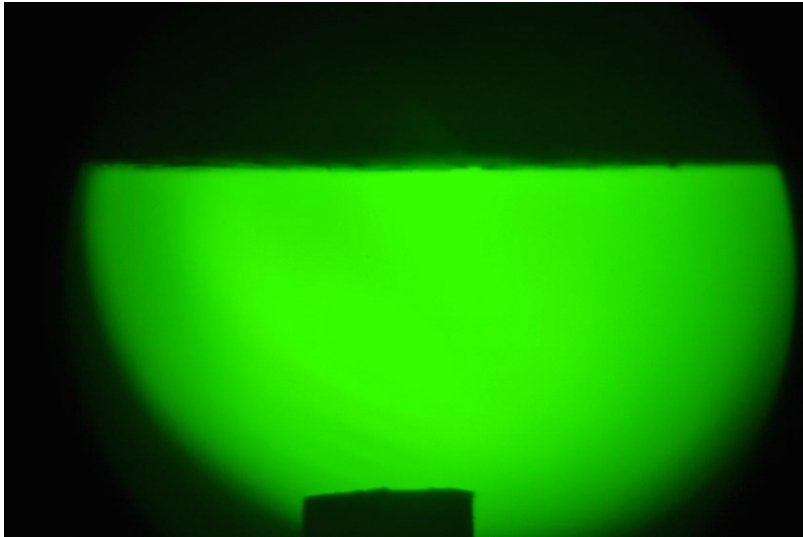
Hydro-Thermo-Mechanics

Experiments

- Static contact angles
- Dynamic contact angles
- Relative permeabilities

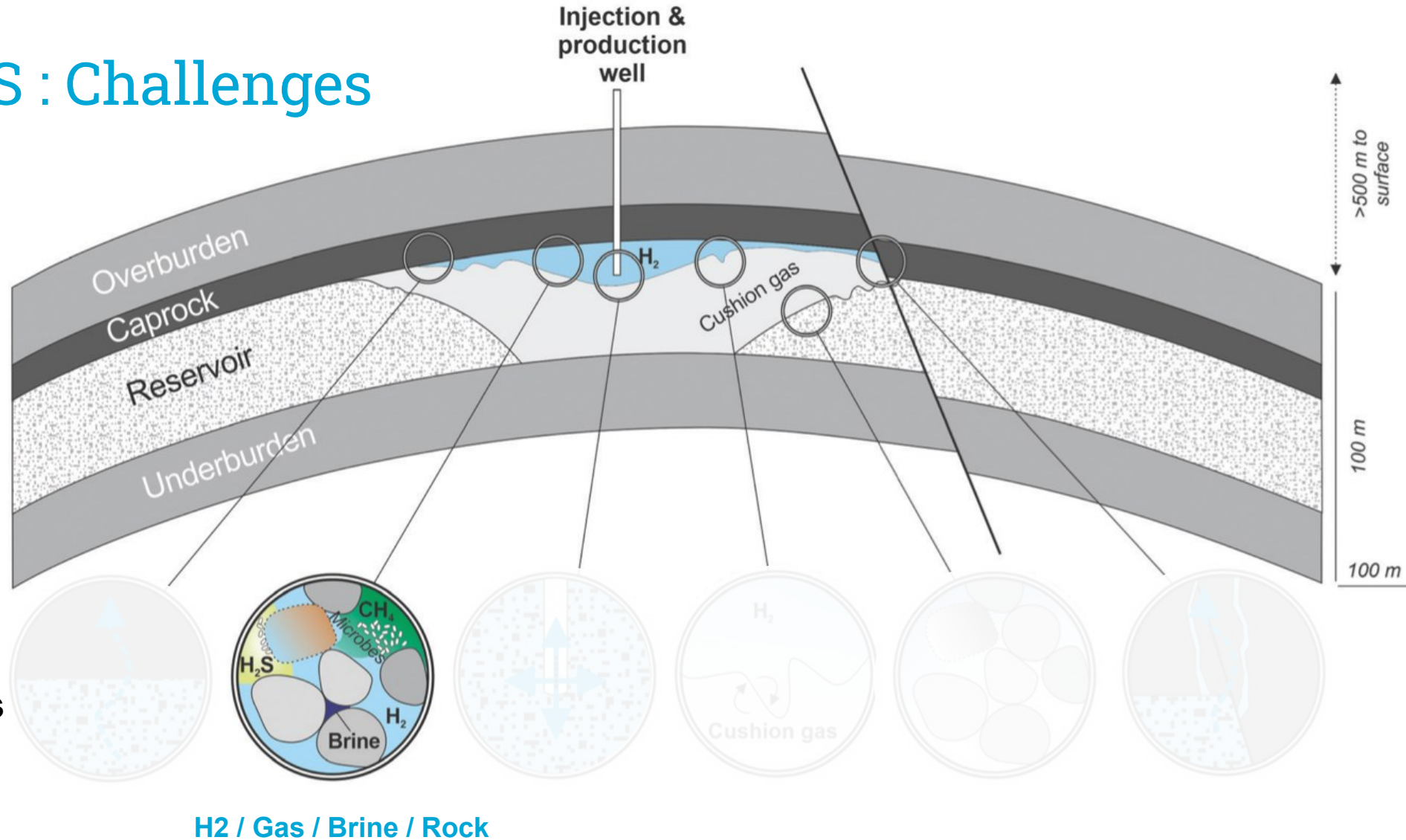
Enabling large-scale hydrogen storage in porous media – the scientific challenges, Heinemann et al., *Energy Environ. Sci.*, 2021, **14**, 853

H₂ / Water / Sandstone : Static contact angles



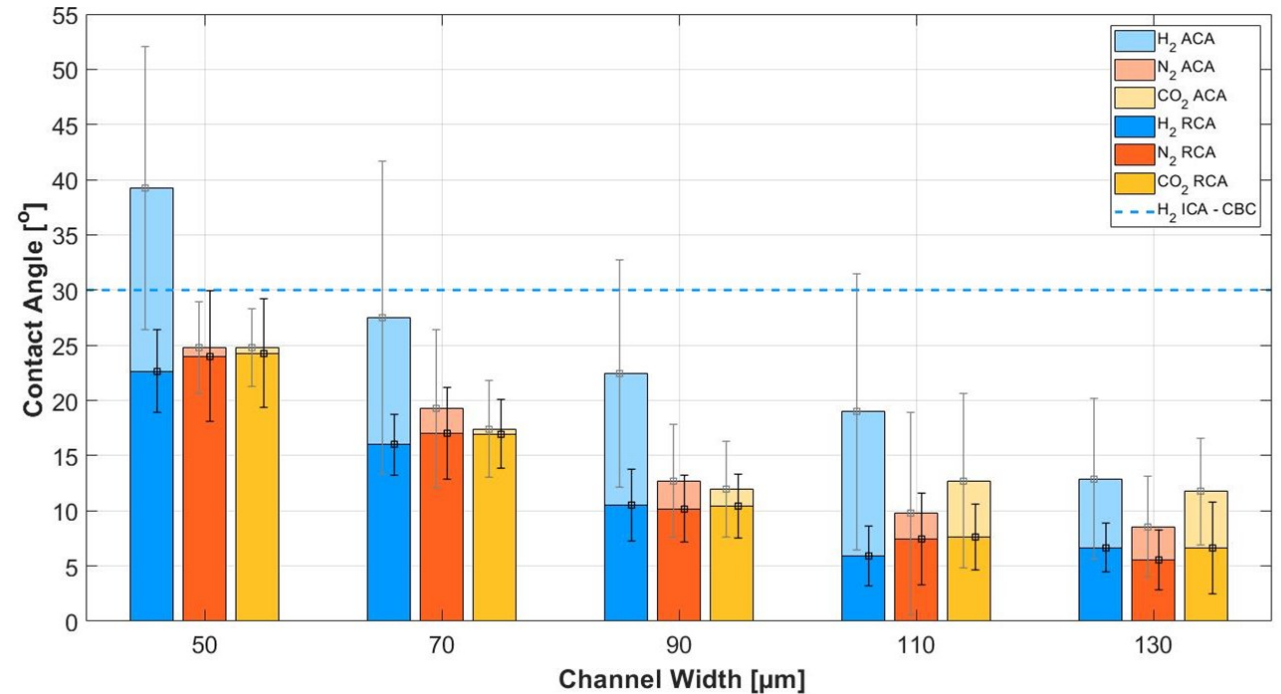
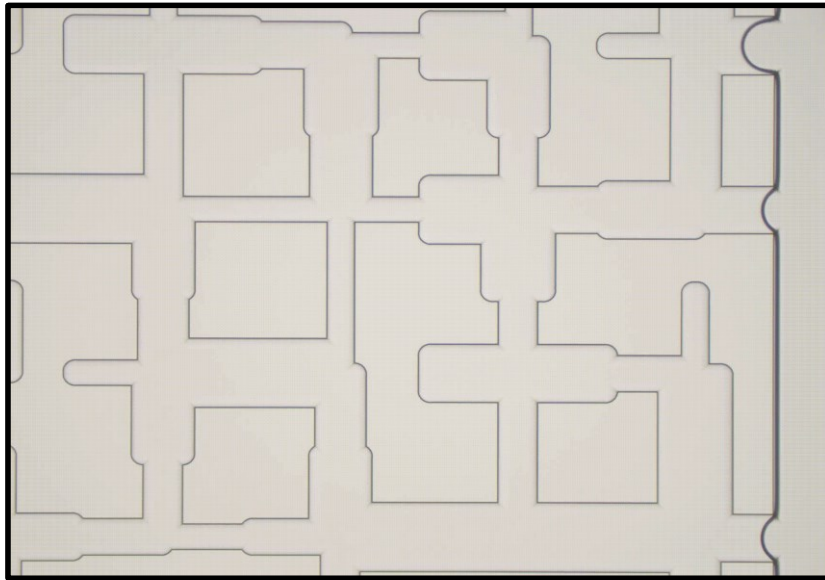
- Measurement of static contact angles for Hydrogen / Brine / sandstone using captive bubble cell
- Wetting angles independent of P , T and salinity ; A theoretical validation based on Young-Laplace Equation
- Hashemi et al., Adv. Water Res. 2021, <https://doi.org/10.1016/j.advwatres.2021.103964>
- Hashemi et al., Adv. Water Res. 2022, <https://doi.org/10.1016/j.advwatres.2022.104165>

Enabling UHS : Challenges



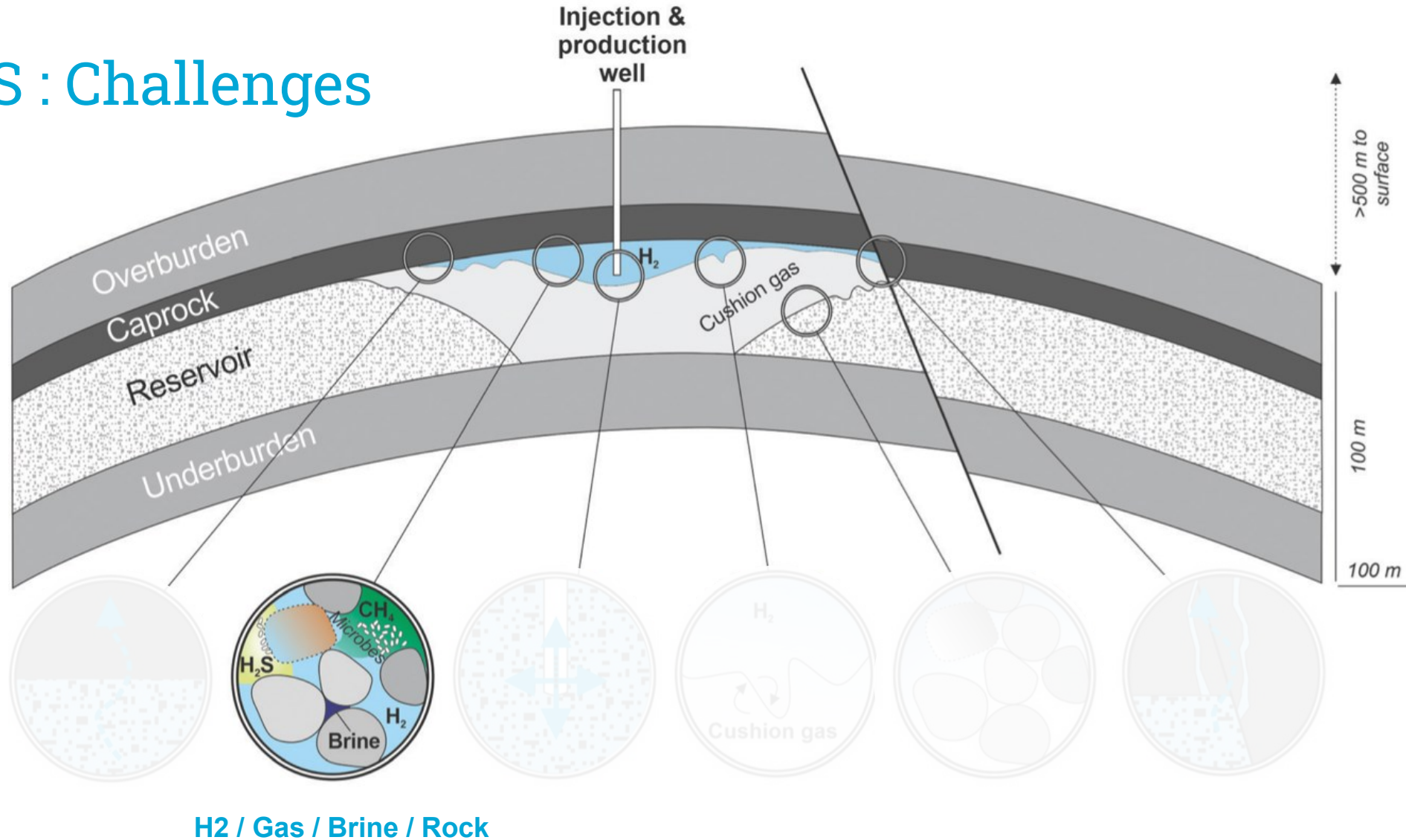
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H₂ / Water / Glass : Dynamic contact angles



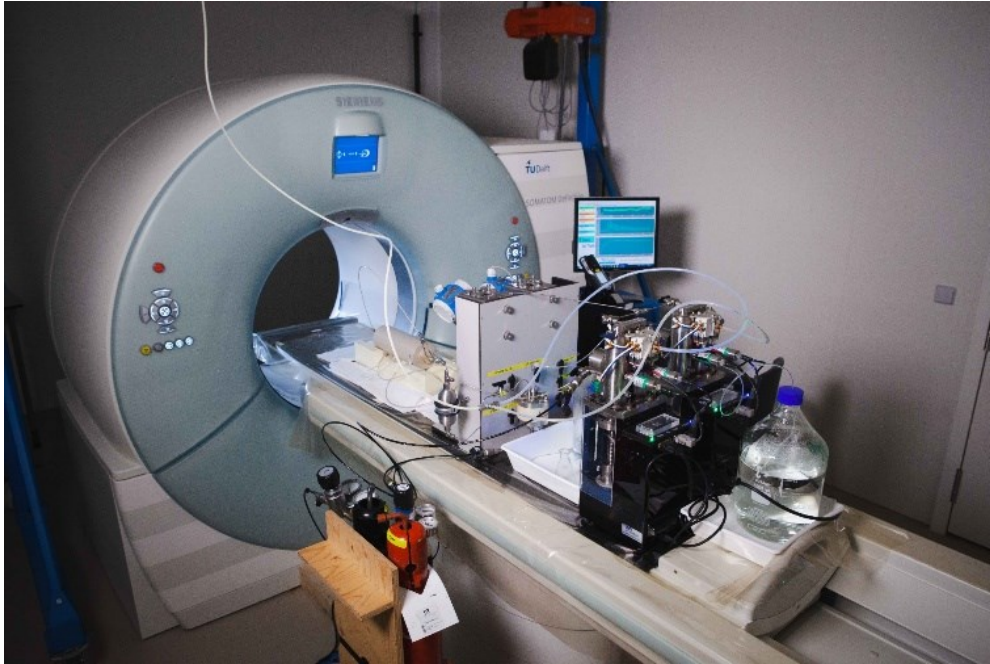
- Measurement of dynamic contact angles for Hydrogen / Brine / Glass using microfluidics
- Dynamic contact angle decreases with channel width ; Similar behaviour for CO₂ and N₂
- Van Rooijen et al., Adv. Water Res. 2022, <https://doi.org/10.1016/j.advwatres.2022.104221>

Enabling UHS : Challenges

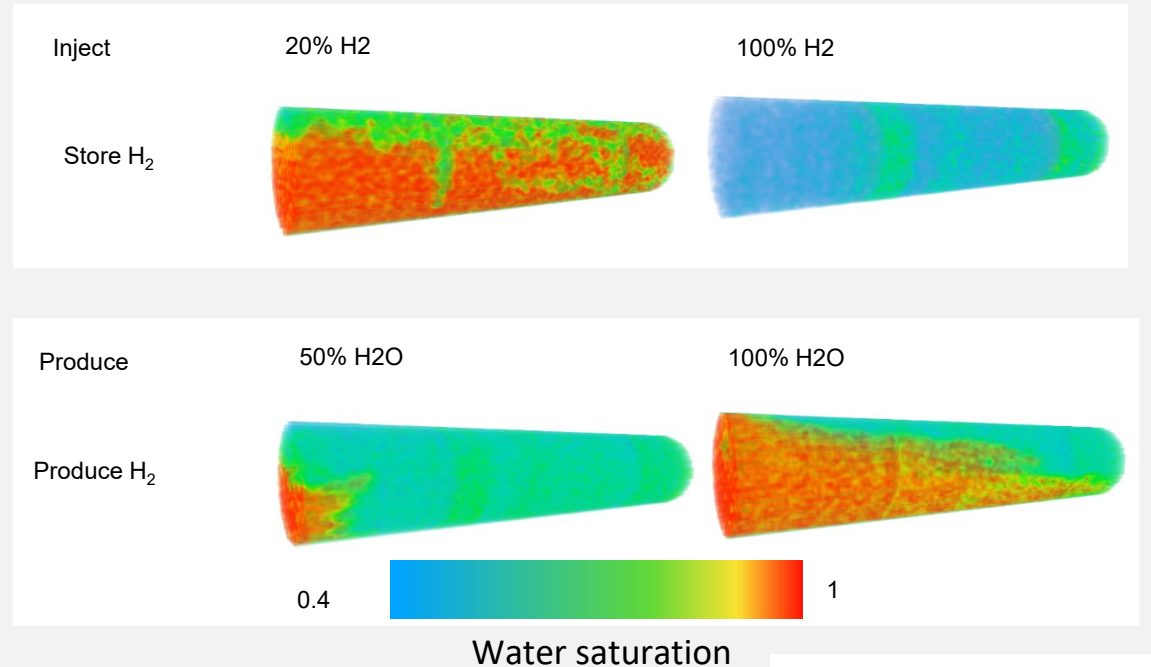


Enabling large-scale hydrogen storage in porous media – the scientific challenges, Heinemann et al., *Energy Environ. Sci.*, 2021, **14**, 853

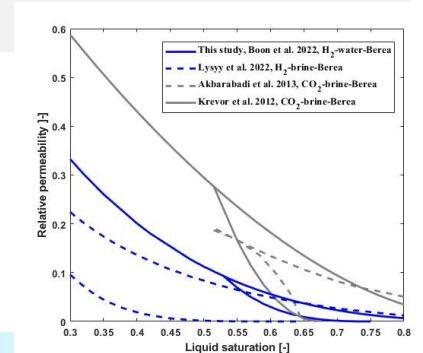
H₂ / Water / Rock system micro-scale transport visualisation



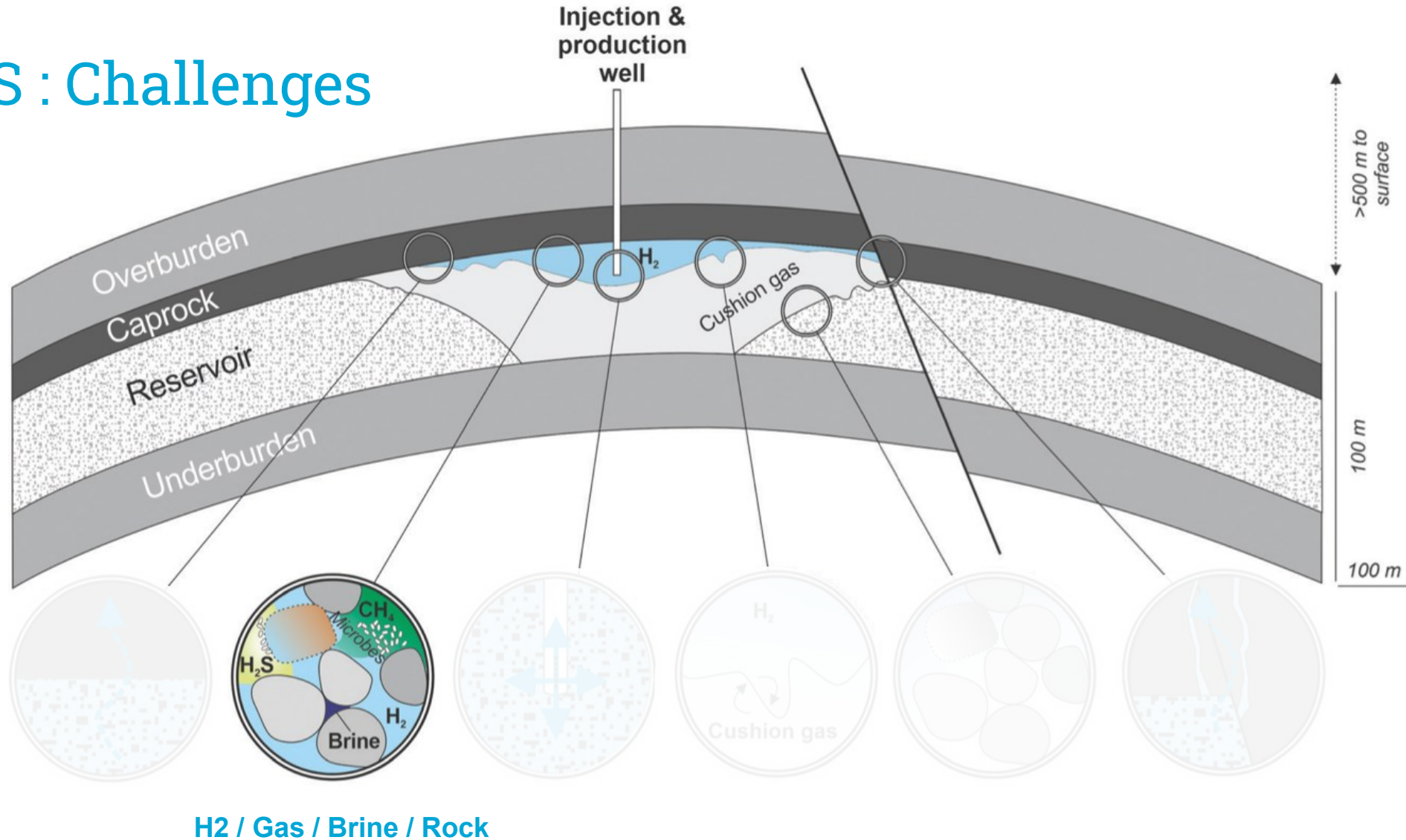
Boon & Hajibeygi, *Sci. Rep.* 2022, <https://doi.org/10.1038/s41598-022-18759-8>



- The first ever core-flood experiment of H₂/Water under CT, visualized H₂ transport
- Found: unique H₂-specific features! Hysteretic Pc, Kr curves!
- Boon & Hajibeygi, *Sci. Rep.* 2022, <https://doi.org/10.1038/s41598-022-18759-8>



Enabling UHS : Challenges



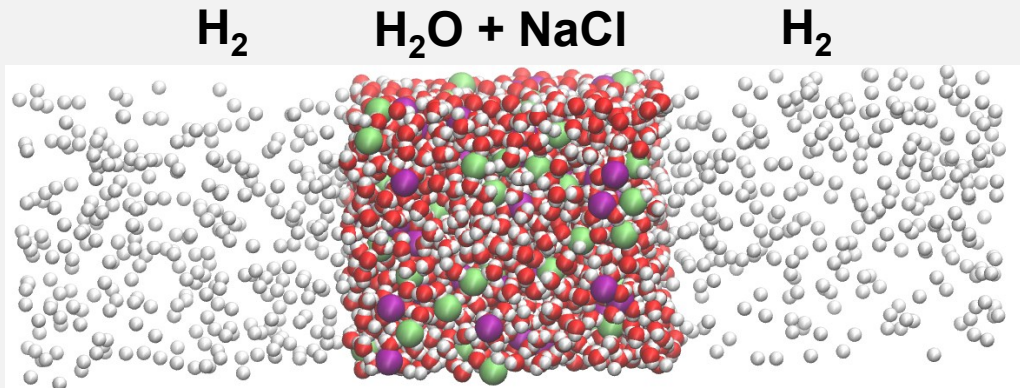
Hydro-Thermo-Mechanics

Molecular Simulations

- Interfacial Tensions
- Solubilities
- Diffusion coefficients

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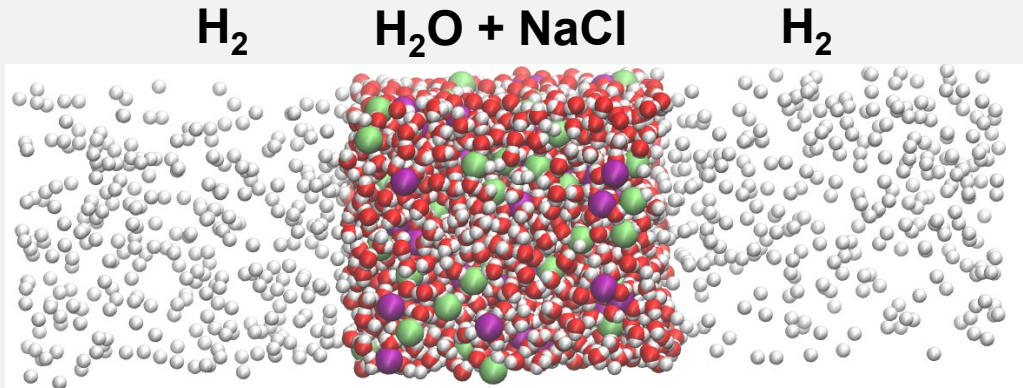
Interfacial Tensions and Transport properties (H₂ – Brine)



Van Rooijen et al.,

<https://doi.org/10.1021/acs.jced.2c00707>

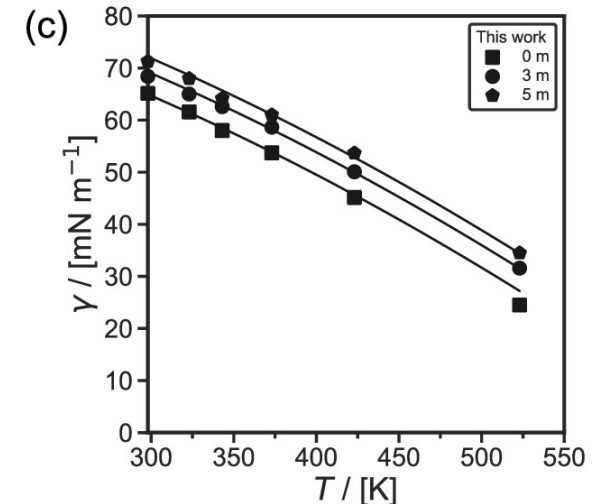
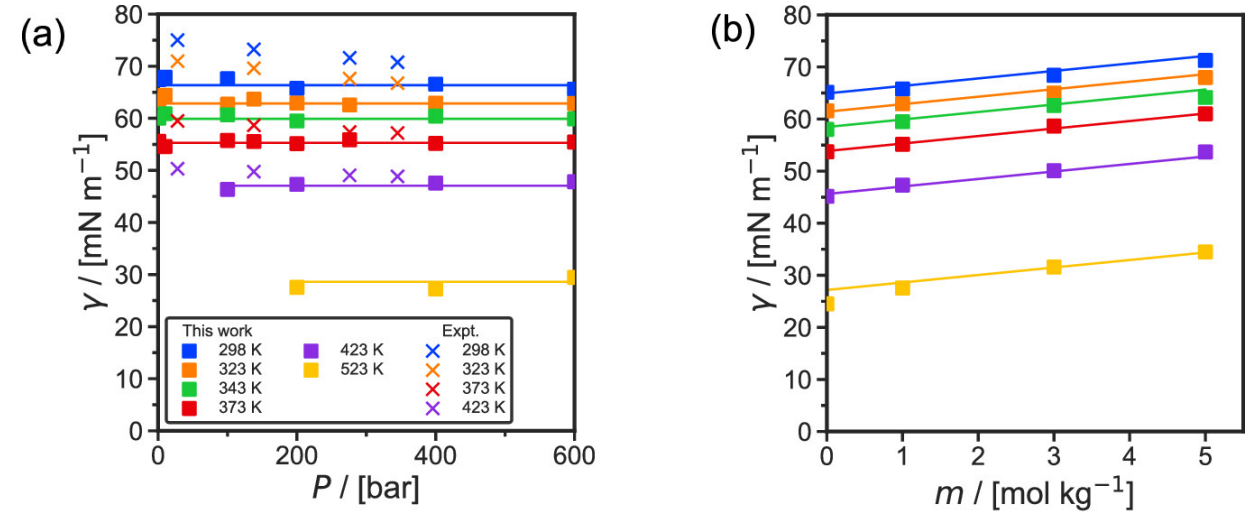
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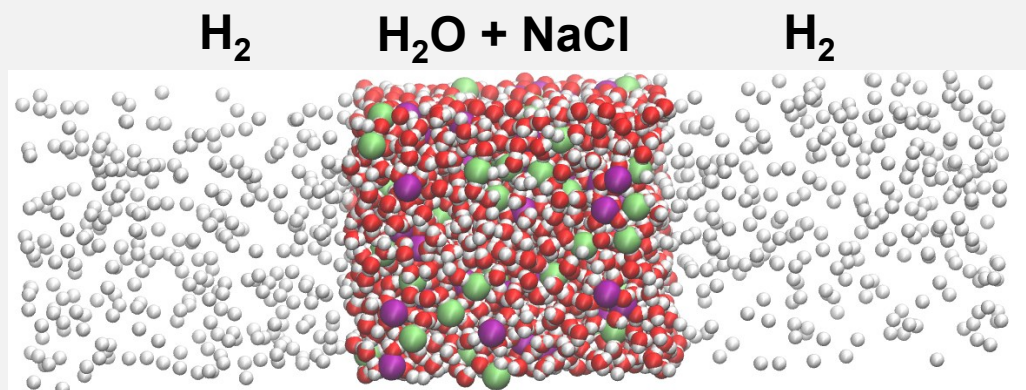
- Interfacial tension of H₂ / Brine at reservoir P, T and salt concentration

Van Rooijen et al.,

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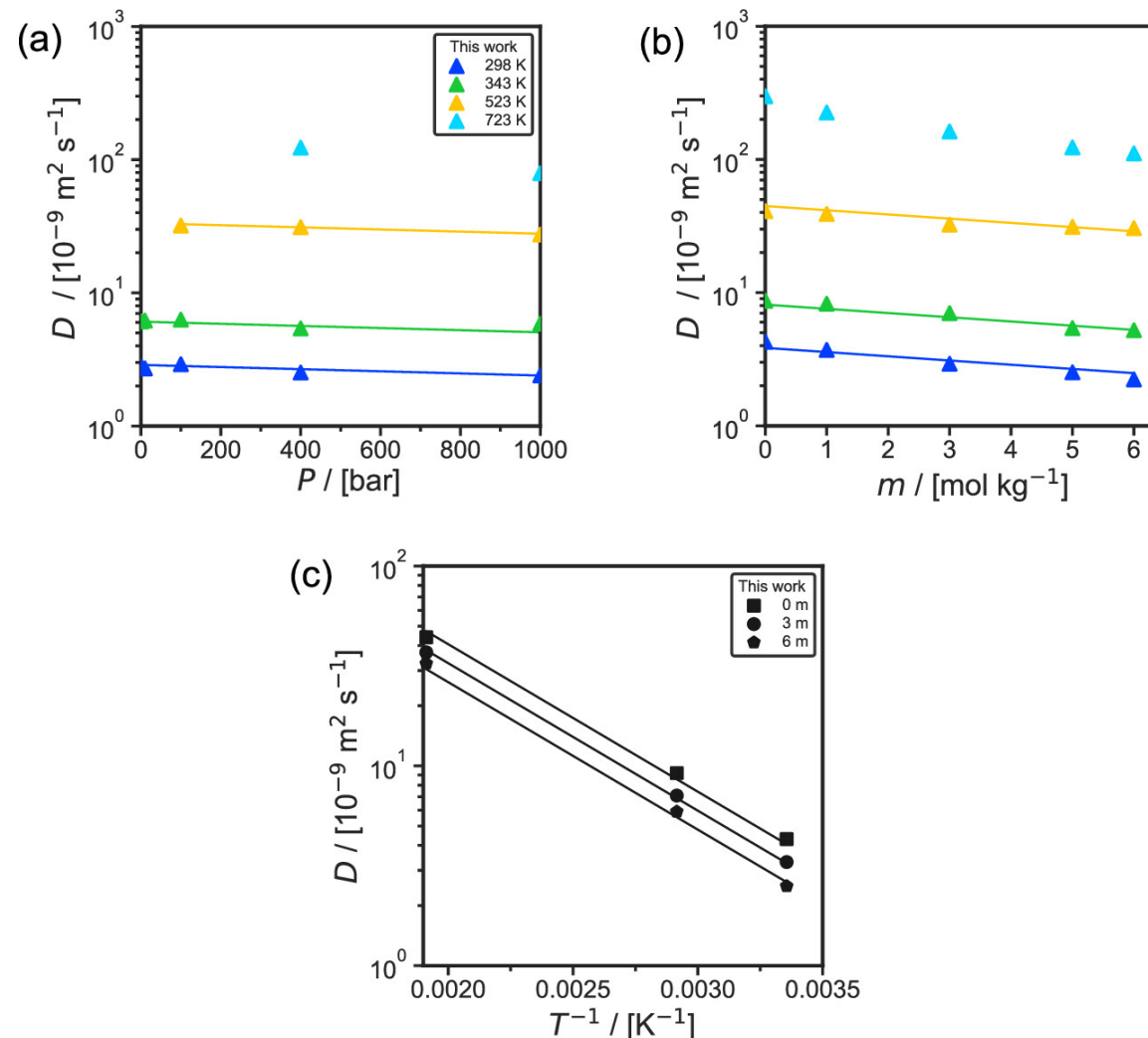
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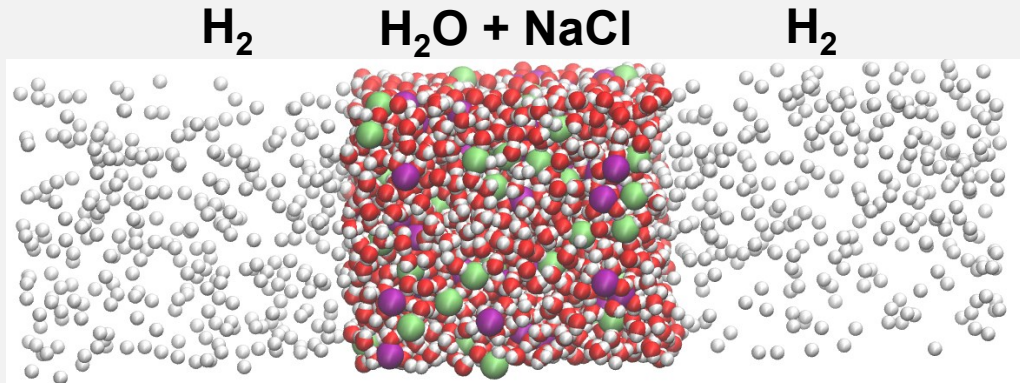
- Interfacial tension of H₂ / Brine at reservoir P, T and salt concentration
- Diffusion coefficients and viscosities of H₂ in Brine solution

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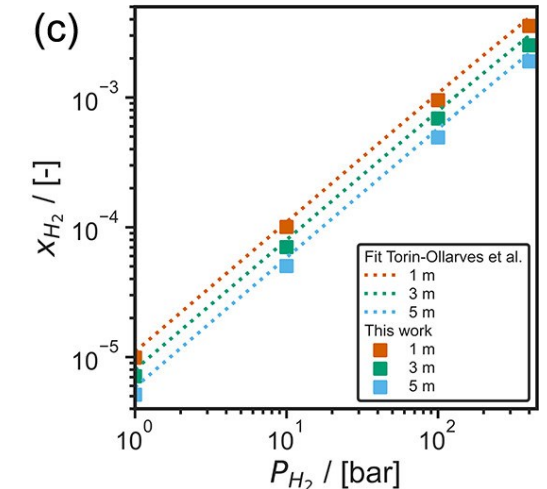
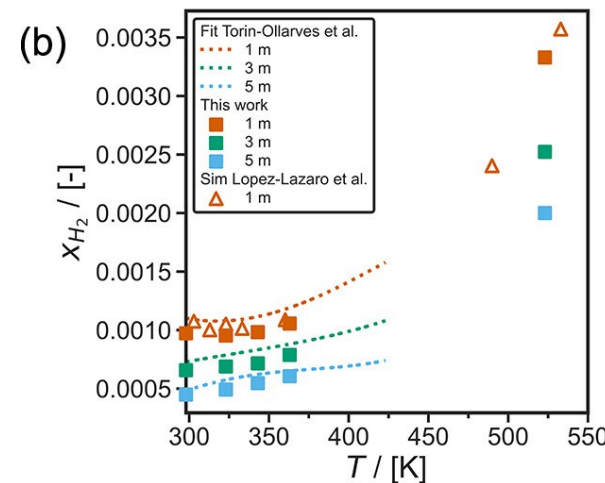
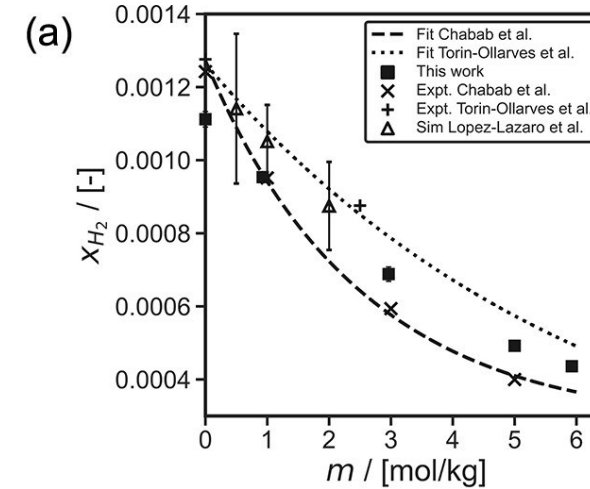
Interfacial Tensions and Transport properties (H₂ – Brine)



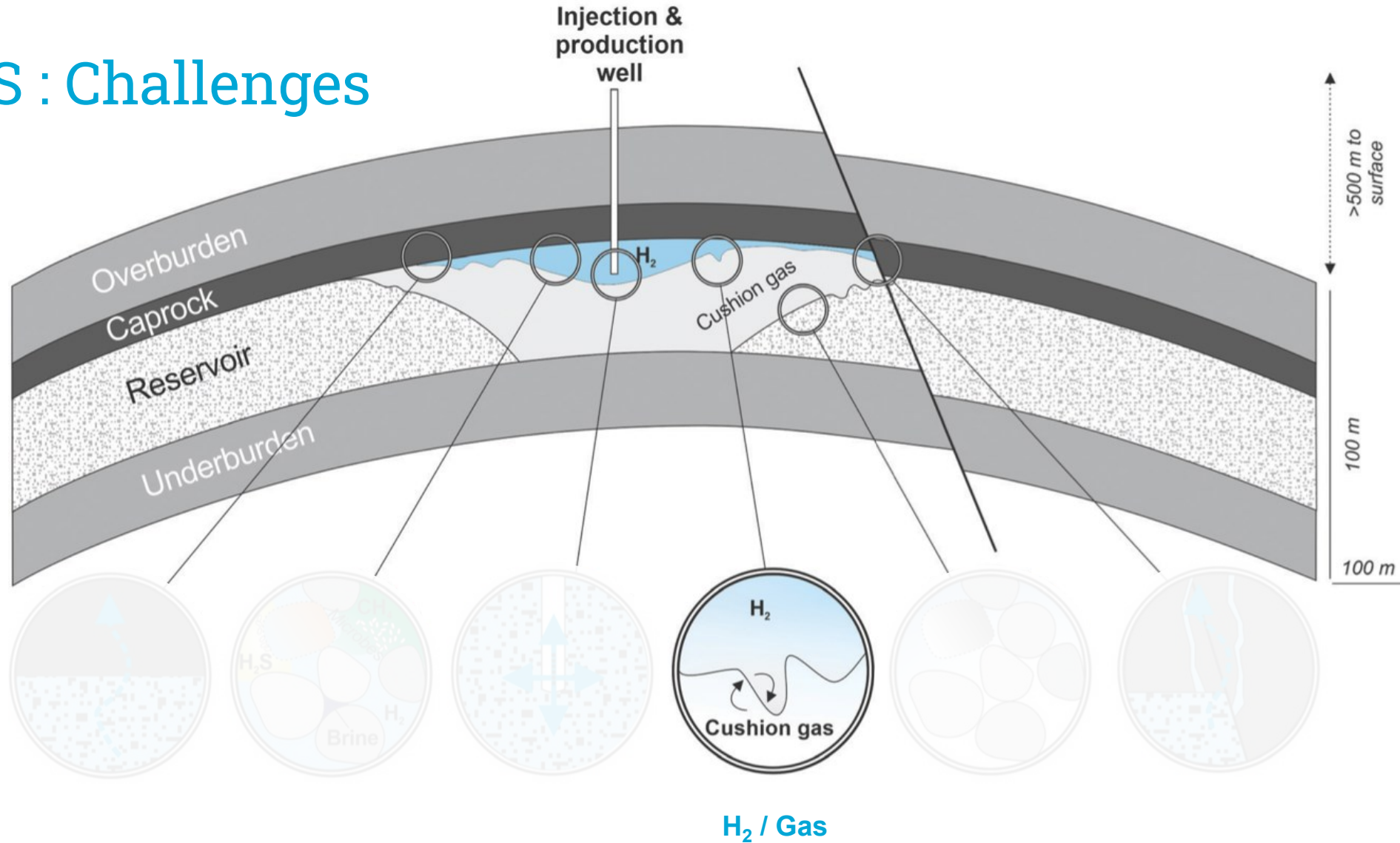
- Interfacial tension of H₂ / Brine at reservoir P, T and salt concentration
- Diffusion coefficients and viscosities of H₂ in Brine solution
- Solubilities of H₂ in Brine solution

Van Rooijen et al.,

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Enabling UHS : Challenges



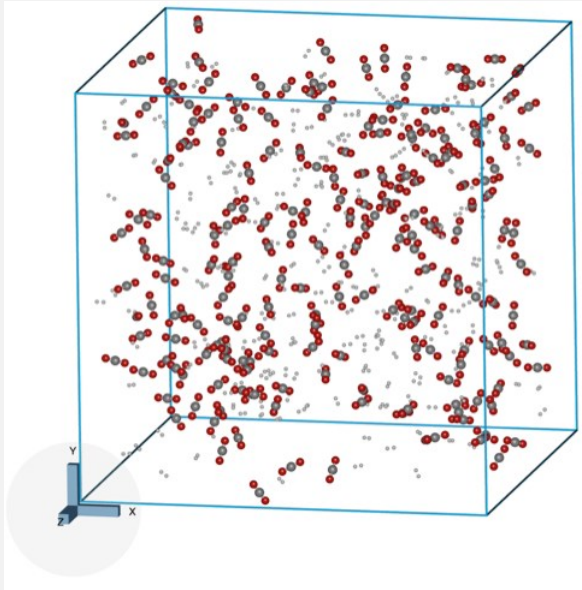
Hydro-Thermo-Mechanics

Molecular Simulations

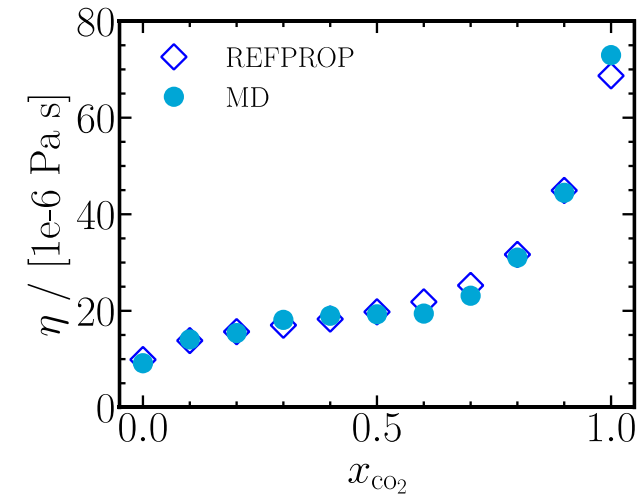
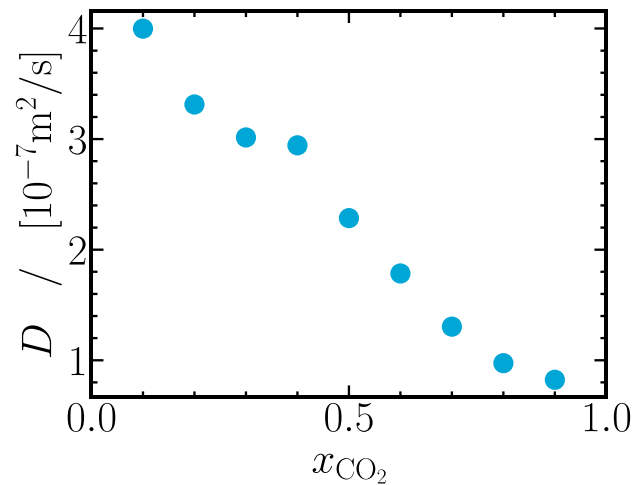
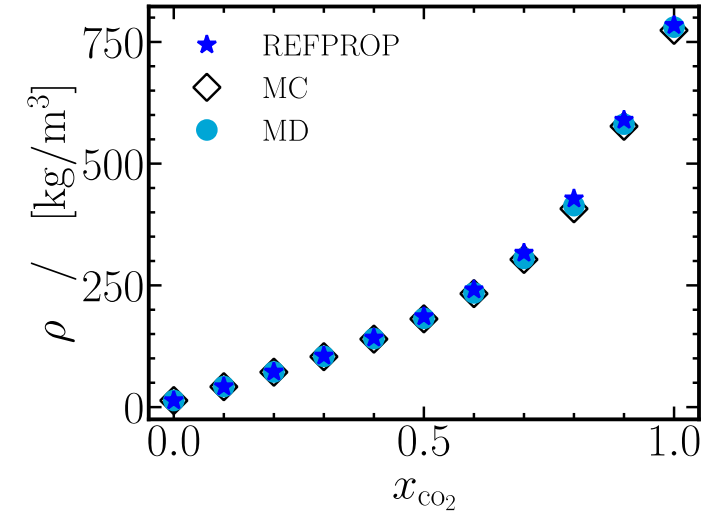
- Diffusion coefficients

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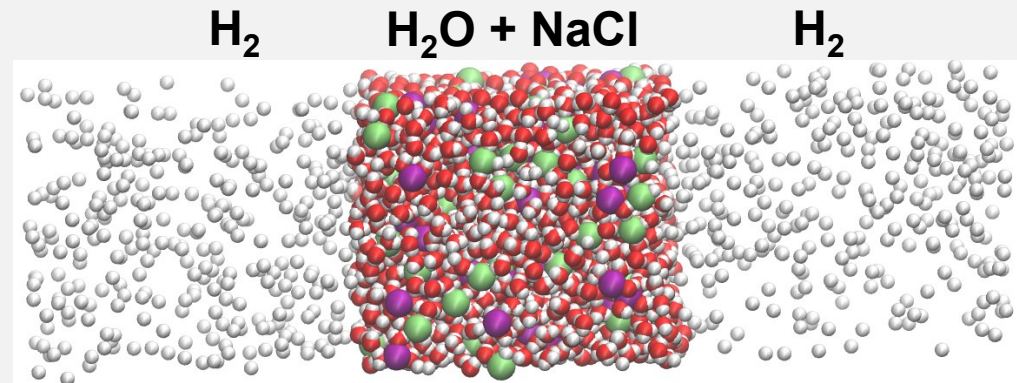
Diffusion coefficients



- Densities, Fick diffusion coefficients and viscosities of H₂-CO₂ mixtures
- Solubilities of H₂-CO₂ mixtures in Brine solution



H₂ Toolbox



H₂ Toolbox : A Molecular Thermodynamics toolbox for H₂ / Brine System

Densities Viscosities Solubilities

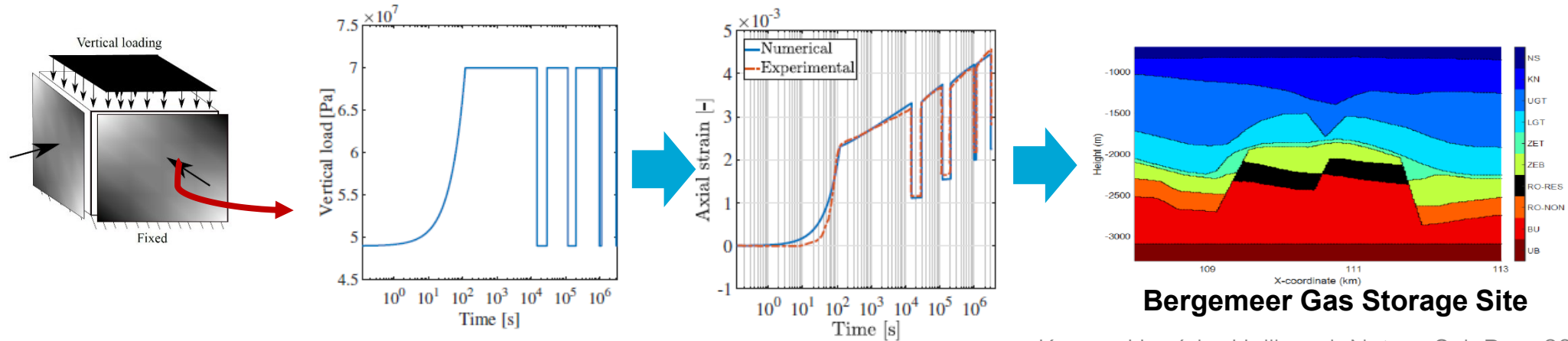
Diffusion-coefficients Contact Angles

Conclusions

- Underground Hydrogen Storage (UHS) is a promising technology
- Challenges in enabling UHS are multiscale and interdisciplinary in nature
- Hydrogen storage (thermodynamically) different in comparison to CO₂ or natural gas
- Extensive characterization still required
- H₂ toolbox developed for thermodynamic properties H₂ of and its mixtures

Other factors

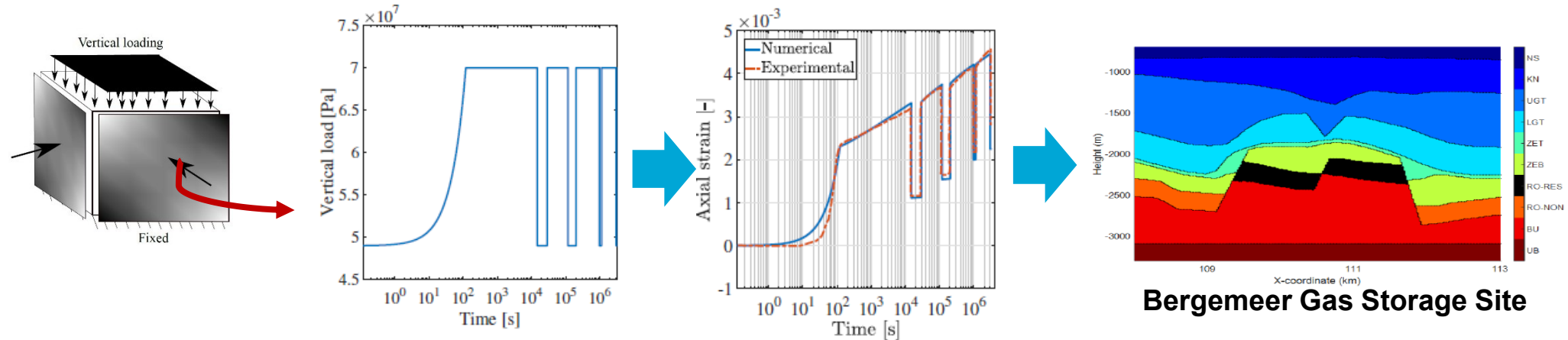
- **ADMIRE project involves much more than hydro-thermodynamics of storage**
- **Specially, geomechanics (storage integrity & efficiency) under cyclic loading**



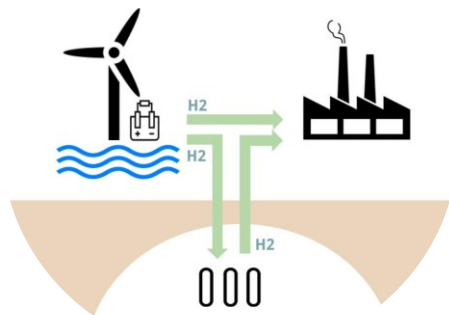
Kumar, Honório, Hajibeygi, Nature Sci. Rep. 2022,
<https://doi.org/10.1038/s41598-022-25715-z>

Other factors

- **ADMIRE project involves much more than hydro-thermodynamics of storage**
- **Specially, geomechanics (storage integrity & efficiency) under cyclic loading**



Kumar, Honório, Hajibeygi, Nature Sci. Rep. 2022, <https://doi.org/10.1038/s41598-022-25715-z>



- **And, techno-economics of storage!**

Storage in Salt Caverns will cost about 10-15% of the production costs!

Eradus, Hajibeygi, Ad van Wijk

<http://resolver.tudelft.nl/uuid:8eb96cf8-2c91-4553-b0cb-a41458f61b5d>

Thank you!

Project Admire (NWO)

ADMIRE & DARSim research team members

Subsurface Storage Theme

TU Delft, Process & Energy researchers

<https://www.tudelft.nl/citg/UHS-SummerSchool>



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Thermodynamics of Storage

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