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The Migration of Hydrogen in Sedimentary Basins

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Abstract

Understanding the mechanisms of large-scale, subsurface hydrogen migration is essential for natural hydrogen exploration and for hydrogen storage assessment. The unique properties of hydrogen make that the timescales of hydrogen migration within geological basins vary from thousands of years to days. Within the shallow Earth, diffusive and advective transport mechanisms are dependent on a wide range of parameters including geological structure, microbial activity, and subsurface environmental factors, e.g., salinity, temperature, and pressure. In this study, we review the nature and timescale of hydrogen migration in geological basins. We also review the mechanisms and timescales of hydrogen migration within diffusive, advective and biologically moderated systems within the shallow Earth. We calculate maximum vertical velocity, $\boldsymbol{v_{max}}$, for several key rock types, including sandstone and micrite and discuss the importance of capillary pressure in controlling the mode of hydrogen migration in sedimentary rocks. Finally, We discuss the potential application of causal analyses methods to constrain complex processes in hydrogen systems and assess the challenges of conventional reservoir modelling for hydrogen migration.

Keywords: basins, causal relationships, hydrogen, earth, migration, modelling, resource, velocity

Introduction

Hydrogen is an important component of the world's transition towards a low emission, net-zero future (Agency 2021). Significant efforts are currently being made across academia and industry to improve our understanding of natural hydrogen occurrence and geological storage (e.g., Zgonnik 2020, Muhammed et al. 2022, Wang et al. 2023). Within the literature, the term ‘natural hydrogen’ describes hydrogen formed by geological, chemical and biological processes in Earth’s crust and sedimentary basins. Following planetary accretion, the stabilisation of liquid water on Earth’s surface and onset of plate tectonics at ~ 3.8 Ga had a profound impact on the dynamics of mantle flow and Earth’s hydrogen cycle. This includes the contamination of non-primitive material into Earth’s mantle at subduction zones and heterogeneous hydrogen distributions within the mantle. Conversely, isotopic signatures show that primitive mantle material delivered to Earth’s surface at hotspot settings preserve their primordial hydrogen and must not mix significantly with surrounding mantle during their ascent (Jimenez-Rodriguez et al. 2023, Jackson et al. 2017, Allègre et al. 1995, French & Romanowicz 2015). Hence,the timescale of hydrogen transport from within the deep Earth to different geological settings at the surface vary across several orders of magnitude, and from billions to millions of years.

Within the shallow Earth, natural hydrogen is encountered as a free gas (i.e., surface seeps), dissolved in groundwater and within fluid inclusions in rocks and migrates through a wide range of mechanisms, including diffusion (e.g., through crystalline lattices) and advection. The passage of hydrogen from Earth’s interior to the surface and atmosphere is dependent on a wide range of factors that relate to the origin of hydrogen, its transport mechanisms and interaction with the materials it moves through. Whilst the hydrogen budget of the deep Earth must have been set during early Earth history, there is a clear dichotomy with shallow Earth process that both generate and consume hydrogen on significantly shorter timescales. Furthermore, unlike other geological fluids commonly considered in Earth Sciences, mass balance cannot be assumed for natural hydrogen systems due to the sheer number of unknown factors within subsurface systems. Hence, these complexities represent critical knowledge gaps in our understanding of subsurface hydrogen migration. Whilst laboratory experiments and assessments of specific case studies have shed some light on the complex nature of natural hydrogen migration, large gaps remain in our understanding of the mechanisms responsible for the migration of hydrogen within geological basins.

In this overview, we review (i) the dynamics of diffusive hydrogen migration, transport along faults and fractures and the role of microbial processes on hydrogen flow within the shallow Earth (ii) review advective hydrogen migration and explore potential modelling approaches for subsurface hydrogen migration.

Hydrogen diffusivity in crystalline and sedimentary rocks

The passage of hydrogen through crustal rocks depends on many factors, including mineralogy, texture and environmental factors. Whilst hydrogen diffusivity decreases exponentially with temperature and increasing grain size in crystalline minerals, imperfections, fractures and crystal size may significantly alter the timescale of hydrogen diffusion from thousands of years to days (Figure 1) (Farver 2010, Demouchy 2010, Li & Chou 2015). Diffusion through micro-crystalline rocks, such as volcanic glasses,

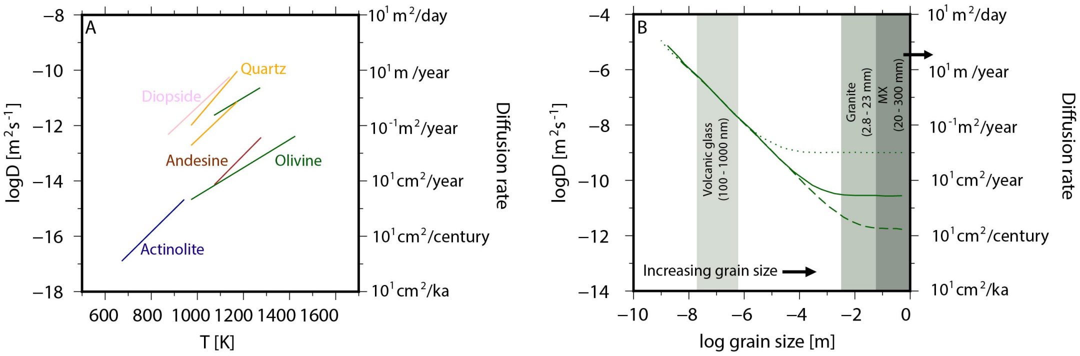


Fig. 1 Hydrogen diffusivity as a function of mineralogy and grain size. A = Hydrogen diffusivity in different mineral structures. Whilst hydrogen diffusivity varies significantly with mineral structure, there is no obvious relationship between the two. B = Hydrogen effective diffusivity in olivine aggregate at 1473 K and 300 MPa and grain boundary width = 0.75 nm (Kohlstedt & Mackwell 1998, Demouchy 2010). Diffusivity decreases exponentially with grain size. Grain size ranges for plutonic granites and mantle xenoliths (MX) are shown in medium and dark grey (Hoskin & Sundeen 1985, Speciale et al. 2020). Black horizontal arrow indicates MX grain sizes beyond the axes range (e.g., Sharapov et al. 2022). Typical grain sizes for microcrystalline volcanic glasses vary from $100 - 1000$ nm and are shown in light grey (Schlinger et al. 1988). Figures modified from (Demouchy 2010, Farver 2010, Li & Chou 2015).

may be instantaneous and thus have important implications for the degassing of mantle hydrogen in hydrothermal and marine settings. For aggregate crystalline rocks such as granites, textural properties typical of ancient cratonic rocks allow hydrogen abundances to be preserved over billions of years and preserve hydrogen concentrations within fluid inclusions, thus creating an important source within the continents (Bourdet et al. 2023, Hutchinson et al. 2024).

Environmental factors, such as temperature, pressure and salinity exert important controls on hydrogen diffusivity in sedimentary rocks. Generally, diffusivity increases with increasing temperature and decreases by several orders of magnitude with increasing salinity and pressure (Li & Chou 2015, Demouchy 2010, Hoskin & Sundeen 1985, Speciale et al. 2020, Liu et al. 2022). A possible explanation for the decrease in hydrogen diffusivity witnessed in experiments due to increasing salinity is the increased connectivity of brine molecules within pore spaces in sedimentary rocks, leading to significantly slower diffusion within water compared to empty pore-space, i.e., air (Strauch et al. 2023). In sedimentary rocks, hydrogen breakthrough times are typically on the scale of years for every metre of rock, however can be exponentially higher ($\sim < 1000$ years per m) for evaporites, e.g., wetted salt (Vinsot et al. 2014, Keshavarz et al. 2022, Bagreev et al. 2004). As temperature and salinity may vary seasonally, such phenomena raise important questions regarding the length of time taken for subsurface rocks, e.g., aquifers, to change from hydrogen barriers to carriers given an influx of low-salinity meteoric water following heavy rains, or vice-versa. Laboratory hydrogen breakthrough times vary significantly with water content, most notably for salt and rocks with micro-pores (e.g., clay), whereby values range from $1 - 843$ hours (Strauch et al. 2023). However, it must be noted that individual bodies of salt will have highly heterogeneous properties with respect to hydrogen migration due to variable fracture density from the centre (lowest) to the edge (highest) where salt is in contact with surrounding sedimentary rock.

Faults and fractures

The advection of hydrogen along faults and fractures represents a significant method of transport of hydrogen to Earth's surface. Several well-known and historical natural gas seeps exemplify the real-time and consistent flow of hydrogen to Earth's surface over the last several millennia, e.g., Mount Olympus, Turkey (Hosgörmez 2007). Such hydrogen seeps are generally associated with deep crustal-scale faults that intersect hydrogen-rich rocks, e.g., serpentinised crystalline basement. In contrast, periodic hydrogen pulses have been attributed to seismically induced groundwater transport along faults, neotectonics and CO_2 migration (Firstov & Shirokov 2005). In regions of active faulting, stress cycling and the creation and destruction of permeability and fluid flow are closely linked. Whilst both large (km) and small-scale ($<$ m) faults are capable of influencing fluid migration pathways within sedimentary basins,the migration of hydrogen across large length-scales is dominated by advection along major faults. The advection of hydrogen-enriched fluids along large-scale faults are attributed to natural hydrogen fluxes recorded in several well-known case studies, including Mali, Brazil and the north Pyrenees (Prinzhofer et al. 2018, Donzé et al. 2020, Lefeuvre et al. 2022). Common factors include the intersection of deep, crustal-scale faults with Archean-Proterozoic crystalline basement or ultramafic mantle bodies that are serpentinised, hydraulic or elevated temperature and pressure gradients that trigger fluid migration. Measured daily flow rates of gaseous H_2 flux within fault zones by Lefeuvre et al. (2022) range from $0.07 - 0.15$ $m^3 m^{-2} d^{-1}$ in the north Pyrenees. These values are comparable to measurements of gaseous H_2 flux within soils from the Sao Francisco basin in Brazil and the Semail ophiolite, Oman (Prinzhofer et al. 2019, Zgonnik 2020, Moretti et al. 2021). The measurements of Lefeuvre et al. (2022) equate to a timescale of $\sim 128 - 274$ years for hydrogen migration over a distance of ~ 7 km from its serpentinite source to trap beneath a clay-rich seal. Hence, faults and fractures present conduits for both long and short-term hydrogen migration from a range of crustal depths to the surface.

Microbes

There is a growing consensus that subsurface microbial communities are independent of photosynthesis for carbon and hydrogen supply, and are primarily or completely dependent on abiotic hydrogen sources in various geological settings as an energy source (Kotelnikova & Pedersen 1998, Takai et al. 2004, Lin et al. 2005, McCollom & Amend 2005, Nealson et al. 2005, Escudero et al. 2018, Gregory et al. 2019). For microbial life to survive, temperature limits must lie between $-15°C$ to $+121°C$, corresponding to depths of up to $3.5 - 4.5$ km beneath Earth's surface at normal geothermal gradients of $30 \pm 5°C\ km^{-1}$ (Dopffel et al. 2021). The rate at which microbial reactions moderate hydrogen flow through rocks or sediments is highly dependent on environmental factors including abundance of air, temperature, salinity and acidity of porefluids and groundwater, abundance of iron and nutrients. For shallow rocks (< 100s m), soil and regolith, environmental signals dependent on surface and near-surface processes will be attenuated on timescales as short as hours to months (e.g., Harris et al. 2007). However, for deep rocks (> 1 km, such as deep saline aquifers) environmental signals may be attenuated over timescales of thousands of years or longer. Hence, the degree to which microbial reactions influence hydrogen migration pathways is dependent on the timescale of response of the microbial host material to environmental change. Shallow systems which are affected by diurnal to seasonal environmental variations will moderate hydrogen flow on these timescales, whereas deeper systems with sufficient nutrients, such as Fe^{3+}, will sustain microbial reactions over longer timescales and be affected by long-term environmental change.

Modelling hydrogen migration

It is clear that the migration pathways of subsurface hydrogen are complex, and that subsurface hydrogen systems will be inherently open with processes operating on an unknown number of variables at vastly different timescales. Traditional schools of thought, including reservoir and groundwater modelling lack many of the key components required for evaluating subsurface hydrogen migration, including sufficiently short timestepping, modelling both past and future processes, accounting for changes in mass balance, phase, solving equations relevant for hydrogen, such as equations of state (EoS) and saturation relationships. Hence, new methods are required to incorporate such complexities into conventional modelling approaches to predict the flowpaths and rate of hydrogen migration in the subsurface.

Estimation of hydrogen velocity

Lodhia & Clark (2022) calculate the maximum vertical velocity, v_{max}, of gas-phase and liquid-phase advection for different geological fluids in sandstone and micrite by applying the multipoint method to define porosity-permeability relationships (see Appendix A in Hantschel & Kauerauf 2009) and estimation of connate water saturation as a function of porosity and depth using Athy's relation (Athy 1930, Holmes et al. 2009). Parameters for EoS, geothermal gradient, surface temperature and pressure regime (e.g., normal, hydrostatic, overpressured) may also be set. We apply this method to estimate the maximum vertical velocity of hydrogen in sandstone, sanstone (clay-rich), micrite and dolomite (Figure 2). Normal values for geothermal gradient of 25°C and pressure-temperature regime of 0.5 MPa K^{-1} are used. As Lodhia & Clark (2022) only consider pure H_2, v_{max} values represent gas-phase advective migration velocities, as hydrogen cannot be a liquid under terrestrial conditions.

v_{max} values for hydrogen vary by an order of magnitude between sandstone and sandstone (clay-rich), and are $\sim 3.8 - 1.5$ and $\sim 0.4 - 0.1$ m $year^{-1}$ between depths of $0 - 2$ km, respectively. v_{max} values for hydrogen vary by several orders of magnitude between dolomite and micrite, and are $\sim 350 - 147$ and $\sim 2.8 - 0.83$ m $year^{-1}$ between depths of $0 - 2$ km, respectively.

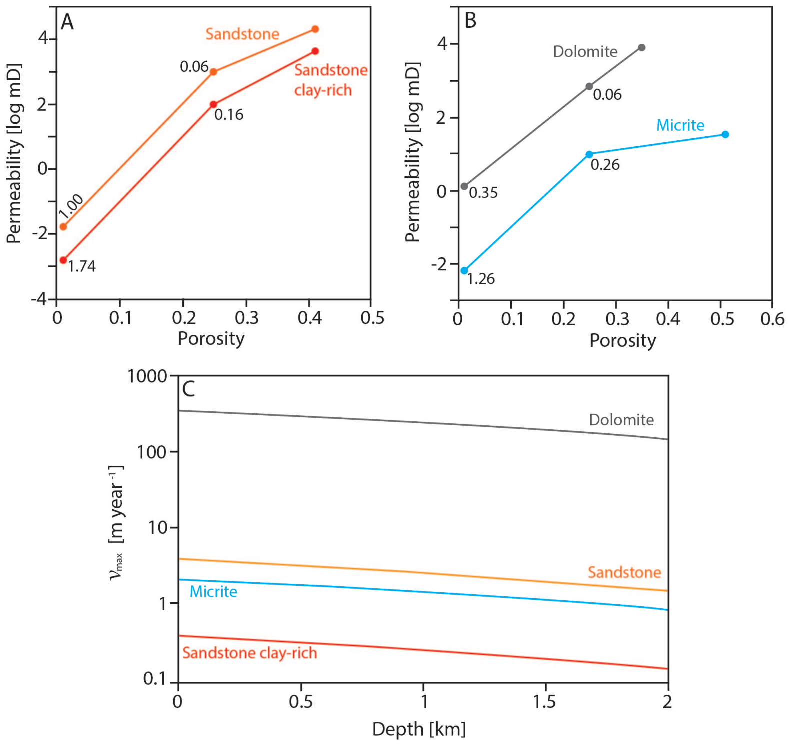


Fig. 2 Porosity-permeability relationships and maximum vertical velocity, v_{max} calculations for various lithologies. A = porosity-permeability relationships for sandstone (typical) and sandstone (clay-rich) and capilary entry pressures in MPa (numbered points). B = porosity-permeability relationships for micrite and dolomite and capilary entry pressures in MPa (numbered points). Data from Hantschel & Kauerauf (2009). C = v_{max} calculated using the method of Lodhia & Clark (2022) for various lithologies versus depth.

Challenges with conventional modelling approaches

The ability to model the passage of hydrogen through sedimentary and geological basins is a critical component of resource mapping and underground storage assessment. However, whilst spot measurements of hydrogen emission from surface seeps are increasingly reported in the literature, there remains no standardised method to predict pathways and timescales of subsurface hydrogen flow. Traditionally, the main fluids of economic interest in Earth's crust are hydrocarbon fluids and groundwater. The former is within the realm of petroleum geology, whilst the latter is within the realm of hydrology. Petroleum systems, reservoir and groundwater modelling are the dominant methods applied to predict the migration of petroleum fluids and groundwater through the subsurface, respectively. Whilst research in these two fields seldom meet, it is important to understand the limitations of each and possible value that may be attained by bridging the gaps between them in order to apply such techniques for modelling hydrogen migration.

By definition, petroleum systems models assess the generation and migration of hydrocarbon fluids in the past, with the aim of predicting the locations of present-day accumulations. The resource potential of hydrocarbon systems is dependent on several key geological and environmental factors, including source rock total organic content, thermal and burial history, timing of migration and seal integrity. However, hydrogen may be sourced from both fossil (e.g., mantle-derived) and generative processes (e.g. biogenic, serpentinisation) and mass balance cannot be assumed, representing a key difference with petroleum systems modelling. Current petroleum systems modelling techniques rely on the application of Equations of State (EoS) and porosity-saturation relationships developed for hydrocarbons, and are not applicable to model hydrogen migration. Reservoir models calculate the flowpaths of hydrocarbon fluids by assuming Darcy-type flow through porous media, and solving equations repeatedly in gridded computational meshes that represent subsurface geological structure. Increased geological and structural complexity leads to a larger number of grid cells, and reservoir models may quickly become computationally expensive to run. Groundwater modelling workflows traditionally include conceptualisation, model run, calibration, uncertainty and sensitivity analyses. Information on aquifer geometry and model domain, boundary conditions, aquifer parameters (e.g., transmissivity, storativity etc.), groundwater recharge, sources and sinks are required to build a conceptual groundwater flow model (Dassargues 2019). Upon defining a conceptual problem, modelling approaches vary from physical, analogue to mathematical models. Physical models involve building and evaluating laboratory models (e.g., sand tanks), whilst analogue problems involve solving boundary value problems that combine the Darcy flow equation and mass balance. However, conventional groundwater models rely on the assumption of mass balance, which cannot be assumed for hydrogen systems.

Given that many, if not most of the assumptions relied upon in traditional petroleum systems and groundwater modelling do not hold for hydrogen, and the complexity of conventional reservoir modelling, the challenge to model subsurface hydrogen migration whether for exploration or storage purposes, is immense. The greatest risks in attempting to model subsurface hydrogen migration will undoubtedly include failing to acknowledge key parameters or processes that may affect the passage of hydrogen through geological media, or using incomplete or no data to constrain problems.

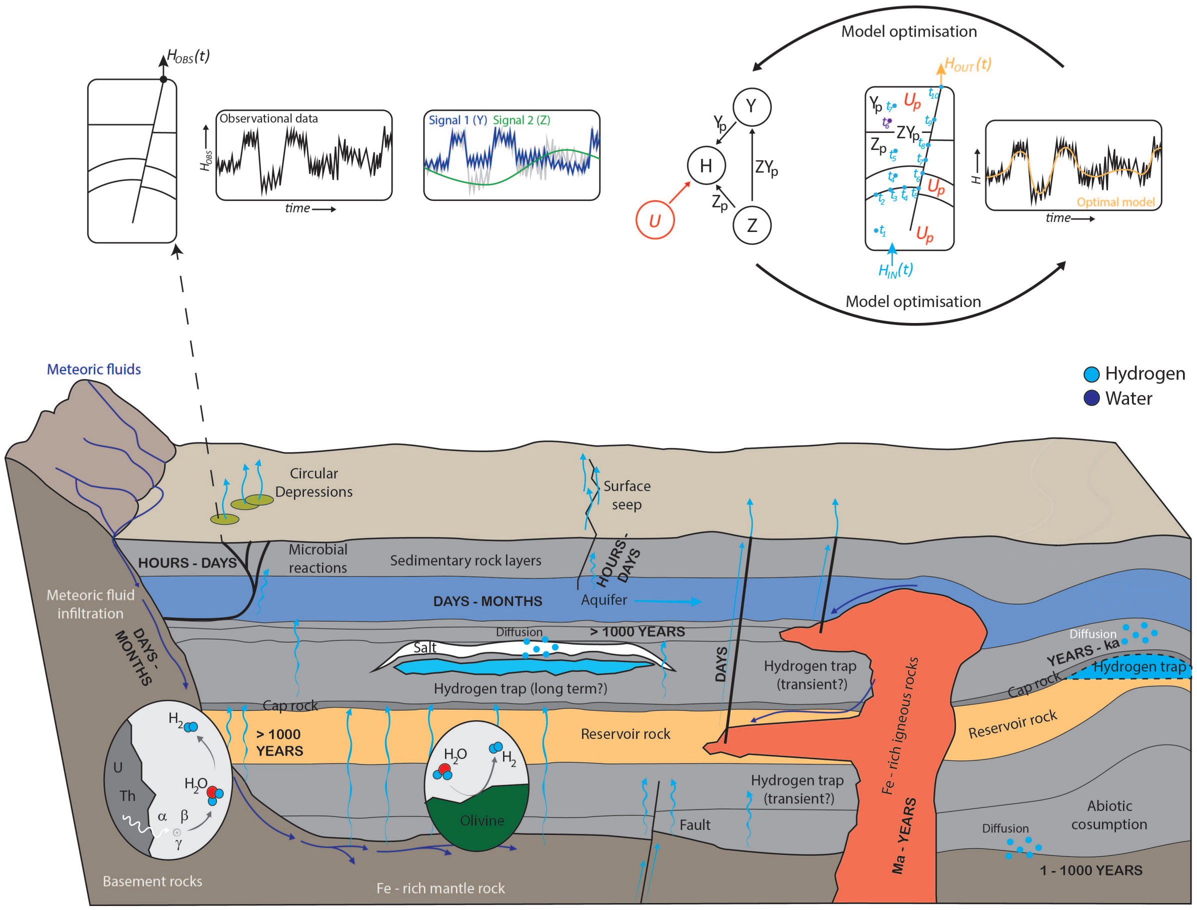
Causal analysis and migration

The shortcomings of conventional modelling approaches highlight the fundamental principle of causality in Earth Sciences: how does one change affect another? In other areas of Earth Sciences with large numbers of unknown, time-dependent factors, such as climate, ocean and atmosphere, correlation and regression methods dominate the modelling space. However, such methods fail to account for unknown variables and process, may be ambiguous to interpret and often lead to incorrect conclusions (Runge et al. 2019). Understanding chains of causes and effects, known as causal pathways, for subsurface hydrogen migration is a daunting task for which various methods of causal inference may be applied. Causal inference is the process of determining the independent, actual effect of a particular phenomenon that is a component of a larger system (Pearl 2009). Runge et al. (2019) summarise methodological challenges for causal discovery in complex spatio-temporal systems, which is undoubtedly highly relevant to subsurface hydrogen. Geoscientific time series, such as hydrogen flux measurements taken at a surface seep, will contain signals from processes acting on vastly different timescales e.g., diurnal pertubations due to microbial activity and long-term hydrogen supply fluctuations caused by changes subsurface environmental factors such as salinity, pH or serpentinisation rates (see schematic diagram of geological time-series data in Figure 3). Surface observations such as flux data may need to be disentangled to better understand causal links and identify key variables and processes. In this way, physical constraints may be used to regularise causal inference methods, e.g., by defining variables (see causal network diagram in Figure 3), restricting functional classes, identifying expected noise distributions, time lags and time aggregation, or general data processing (Runge et al. 2019). We suggest that future work focuses on incorporating information from real experiments on subsurface systems for data-rich case studies and allowing for the combination of observational causal inference and physical modelling of hydrogen migration, and model runs (see top of Figure 3). The combination of causal inference methods with mainstream computational fluid dynamic modelling will be advantageous, as redundant processes may be identified and removed from the modelling workflow thus reducing computational burden.

Discussion

The migration of hydrogen through the subsurface is a topic seldom addressed directly, yet is critical for exploration and geological storage investigations. To understand the dynamics of the subsurface hydrogen cycle within sedimentary basins and Earth's surface, we must take a holistic view of its supply, emission and intermediate processes. Figure 3 summarises the characteristic migration timescales for hydrogen transport through different parts of a sedimentary basin and modelling challenges. Long-term hydrogen supply from the radiolysis of water within crystalline basement, Archean - Proterozoic cratonic rocks and other hydrogen abundant mafic igenous rocks will remain steady over geological timescales. However, within sedimentary basins and Earth's crust, hydrogen migration pathways will be disproportionately affected by specific processes operating within small regions, such as microbial reactions in soil or regolith, advection of fluids along faults and 'trapping' on timescales relative to humans by wet or evaporitic sediments. Environmental factors, such as salinity and temperature may change the dynamics of subsurface hydrogen systems rapidly, for example a saline aquifer changing from a barrier to a carrier due to an influx of fresh meteoric water following heavy rainfall. Hydrogen supply rates within generative systems will be primarily controlled by the availability of fresh water, such as rainfall on ophiolitic systems or groundwater contact with buried igenous rocks.

Within subsurface systems, hydrogen will migrate through porous media by advection in the gas-phase, advection in solution and diffusion, with all three processes occurring as maximum solubility levels are breached at lower temperatures and pressures. A comparison of relative column heights of hydrogen, helium and methane against a nominal fracture gradient of 15.83 kPa m^{-1} is shown by Hutchinson et al. (2024), and highlights that maximum column heights for hydrogen and helium are only marginally less than those of methane. In comparisson to methane, hydrogen is approximately twice as mobile, almost three times more diffuse and significantly less



Challenges

Process:
1 Autocorrelation
2 Time delays
3 Nonlinear dependencies
4 Chaotic state-dependence
5 Different timescales
6 Noise distributions

Data
7 Variable extraction
8 Unobserved variables
9 Time subsampling
10 Time aggregation
11 Measurement errors
12 Selection bias
13 Discrete data
14 Dating uncertainties

Conceptualisation/statistical:
15 Sample size
16 High dimensionality
17 Uncertainty estimation

Fig. 3 Conceptual method for modelling workflow, migration and indicative timescales through sedimentary basins. Bottom: Blue arrows indicate advective transport of hydrogen. Fe-rich lithologies (e.g. granites) characterise Archean - Proterozoic continental crystalline basement within cratonic regions and igneous intrusive rocks. Diffusion through geological barriers to hydrogen migration, e.g. salt and igneous intrusions may limit hydrogen migration by thousands to millions of years, depending on mineralogy and lithology (Farver 2010, Parnell & Blamey 2017). Top: Conceptual diagram showing combination of causal inference, physical modelling and model optimisation. Hypothetical time-series data, e.g. hydrogen concentration measurements ($H_{OBS}(t)$) at a surface seep, may be deconstructed to identify constituent signals Y and Z, operating at different timescales. The causal graph shows the relationships between known variables Z and Y, known causal relationships Z_P, Y_P, ZY_P, unknown variable U and unknown causal relationship U_P. Causal discovery may be used to help design computationally expensive physical model experiments more effectively by identifying key variables and relationships to be included. See Runge et al. (2019) for detailed description of challenges associated with causal inference methods. Modified from Hand 2023, Runge et al. 2019

Property	Description	Reference
Mobility, μ	$\mu_{h_2} \sim 2\mu_{CH_4}$	Lodhia & Clark (2022)
Diffusivity, D	$D_H \sim 2.8 D_{CH_4}$ and $\sim 0.7 D_{He}$ at $25°C$	Montel et al. (1993), Nelson & Simmons (1995)
Solubility, S	$S_{CH_4} \sim 14 S_{H_2}$ at surface	Kaye & Laby (1986)

Table 1 Comparisson of hydrogen properties with methane and helieum.

soluble in water (Table 1, Lodhia & Clark 2022, Nelson & Simmons 1995, Montel et al. 1993, Kaye & Laby 1986).

The results of Hutchinson et al. (2024) indicate that pore throat diameter, and therefore capillary entry pressure, exert a primary control on the mode of hydrogen migration, with increasing advective dominance at larger pore throat sizes (i.e. sandstones) and increasing diffusive dominance at smaller pore throat sizes (i.e. shales, evaporites). Whilst accounting for variable temperature, pressure, fluid chemistry, EoS, lithology and upscaling, the methods used by Lodhia & Clark (2022) rely on relative permeability and water saturation relationships for oil-water and oil-gas that are commonly applied in basin and reservoir modelling, but which are not designed for hydrogen. Such work, whilst important for providing indicative timescales of hydrogen migration, highlights a clear gap in both the knowledge of hydrogen-fluid properties (e.g. hydrogen-water saturation relationships) and also the lack of integration with conventional and industry standard modelling tools useful for hydrogen exploration and storage investigations. Whilst there is no clear link between v_{max} values presented in this study with porosity-permeability relationships (Figure 2A, B), the inverse relationship between v_{max} and capillary entry pressures at different porosity values is intriguing and consistent with the results of Hutchinson et al. (2024). We hypothesise that pore throat size, and thus capillary entry pressure, exert a primary control on both the mode of hydrogen migration and magnitude of advective hydrogen flow through rocks. This is also supported by the exponential decrease in measured hydrogen diffusivities with grain size reported in the literature (Figure 1B, Demouchy 2010) According to this hyposthesis, the greater degree of variation in v_{max} for H_2 between dolomite and micrite in comparisson to sandstone and sandstone (clay rich) may be explained by the increased difference in capillary entry pressures at constant porosity, respectively (Figure 2C). Advection in the gas-phase by Darcy flow will cease when capillary forces in pore spaces in low-permeability rocks are no longer overcome by buoyancy, whereas advective flow will be re-established if the buoyancy pressure overcomes the mechanical sealing strength of the rock (Hutchinson et al. 2024). Within rocks that are characterised by micro-pores, such as evaporites and shales, diffusion will be the dominant mode of hydrogen migration and will be significantly slower than advective transport mechanisms. However, in micro-crystalline rocks such as obsidian, diffusion across grain boundaries will be several orders of magnitude faster than coarsely crystalline rocks.

Incorporating the complexities of subsurface hydrogen into conventional reservoir modelling to assess natural hydrogen resource and hydrogen storage potential represents a key industrial challenge. Reservoir models will require a large number of grid blocks and be associated with a large number of equations that need to be solved simultaneously, therefore increasing computational time and cost. The velocity of hydrogen migration along a planar seal with a dipping angle α may be calculated by combining values of v_{max} from Lodhia & Clark (2022) and directional vectors. Hence, solution of the Darcy flow equation as a function of depth and lithology as opposed to solving repeatedly in grid cells could offer a computationally inexpensive, albeit limited, means to estimate subsurface hydrogen velocities.

Conclusion

Hydrogen within the subsurface remains elusive. While entrenched into Earth during planetary formation, the exchange of hydrogen between materials is prevalent during subsurface processes at all depths. Significant advances in understanding the distribution and generation of natural hydrogen have been made in recent literature, however large gaps remain in our understanding of large-scale hydrogen migration. The timescale of hydrogen migration throughout sedimentary basins varies from thousands of years to days, and is dependent on a wide range of lithological and environmental factors. Grain size, temperature and fluid salinity exert important controls on hydrogen diffusivity in crystalline and sedimentary rocks. Fluid migration along faults and fractures is controlled by rock properties, subsurface stress regimes and groundwater properties. Microbial reactions moderate subsurface hydrogen flow by altering mass balance on differing timescales related to depth and environmental factors. Future modelling of subsurface hydrogen migration must address the shortfalls in traditional methods of fluid migration, such as petroleum systems, reservoir and groundwater modelling. Adequate timestepping, lack of mass balance and accounting for complex cause-and-effect relationships represent key future modelling challenges. Furthermore, the mode and rate of hydrogen migration within sedimentary rocks may be a dependent on the ability of fluid buoyancy to overcome capillary entry pressure, instead of permeability as currently modelled in traditional reservoir modelling software.

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Declarations

The authors declare no conflicts of interest.

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