

RESEARCH NEEDS IN POROUS MEDIA FOR THE ENERGY TRANSITION

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How to Cite:

Blunt, M. J., Bazylak, A., Brook, M., Muggeridge, A., & Orr, F. M. (2024). Research Needs in Porous Media for the Energy Transition. *InterPore Journal*, 1(1), ipj260424–2. <https://doi.org/10.69631/ipj.v1i1nr14>

RECEIVED: 20 Nov. 2023

ACCEPTED: 18 Dec. 2023

PUBLISHED: 26 Apr. 2024



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ABSTRACT

This commentary provides an overview of research needs in porous media for the energy transition. Its intent is to provide a short survey of possible topics for researchers that could assist in accelerating the transition from a fossil-fuel to a zero-carbon energy economy. It was written to summarize the discussion at the panel session on the energy transition held at the Annual Meeting of the International Society for Porous Media (InterPore) in Edinburgh in May 2023 (<https://events.interpore.org/event/41/>) and has been prepared by the panellists at this event in collaboration with colleagues.

KEYWORDS

Porous media, Energy transition, Electrochemical devices, Geothermal energy, Carbon capture, Carbon storage, Hydrogen storage, Compressed gas storage, Thermal energy storage

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1. INTRODUCTION: WHY WE NEED POROUS MEDIA RESEARCH MORE THAN EVER

The world's energy is still principally provided by fossil fuels such as coal, oil, and gas, which emit carbon dioxide during combustion. To avoid dangerous climate change, a rapid transition towards renewable energy, combined with the capture of continued carbon dioxide, CO₂, emissions, is necessary - this is called the energy transition. Because oil and gas are found underground in porous rock, one of the main applications of the science of flow in porous media, and certainly the reason for significant funding from industry, was to understand and improve hydrocarbon recovery from the subsurface. With the energy transition, it may be thought that both funding for porous media research and its societal relevance may decline. However, the opposite is true.

1.1. The challenge

To affect the energy transition, new technologies need to be developed, the success of which hinges on an understanding of physical and chemical processes in porous media (2). Any realistic pathway to avoid

global warming of greater than 1.5 – 2°C requires the capture and storage (CCS) of CO₂ at the gigatonne (10¹² kg) scale (17): the CO₂ needs to be stored in the subsurface, in porous rock, for thousands of years. Storage at this scale requires an industry that, in terms of the volumes of fluid handled, is of similar size, if not larger, than the current oil and gas industry. Although the science of multiphase flow in porous media applied to oil and gas recovery can be adapted to study the long-term sequestration of carbon dioxide, there are some unique challenges outlined later in this document.

Second, the intermittency of renewables, principally wind and solar energy, means that excess energy generated during sunny, windy periods needs to be stored for dull, still days when energy is required. There are several ways to store this energy. Hydrogen can be generated from excess electricity using electrolysis and can be used directly for heating or producing electricity in generators or fuel cells. Hydrogen can be used much as a natural gas is used today, and it has a significant role to play in fuelling heavy industry and large vehicles. At a global scale, exajoule-scale storage (10¹⁸ J), on the order of gigatonnes on a mass basis, is required; similar to CO₂, this can only be achieved through the use of subsurface porous reservoirs (6, 7). However, unlike CO₂, hydrogen must be injected and withdrawn repeatedly with minimal losses. Other forms of energy storage include compressed gas, which can be stored in the subsurface, and thermal energy (hot and/or cold water), which is usually stored in porous aquifers. Heat energy can also be extracted from underground - the exploitation of geothermal resources as a renewable energy supply is well established in some parts of the world, but it has huge potential globally. However, the management of these thermal resources requires an understanding of flow and heat transport in porous and fractured media.

Finally, manufactured materials in the energy transition themselves involve porous materials. Electrochemical devices, for instance, including fuel cells and electrolyzers, have porous components, including the gas diffusion layer, which must allow for the flow of gases and water, and the catalyst layer where the reaction takes place. Membranes are another type of porous structure which are used in many applications, including the separation of carbon dioxide from other gases, or to purify a hydrogen stream. Here research can move beyond the hitherto rather restricted scope of characterizing and predicting the behavior of natural systems, to designing the pore structure, wettability, chemistry, and physical properties of the manufactured porous materials so that they offer optimal performance.

1.2. New technology

The rapid development of new tools has revolutionized our understanding of flow and transport processes in porous materials, including three-dimensional imaging at a range of spatial and temporal scales, advances in numerical modelling, and, most recently, the explosion in the use of machine learning. Consequently, the science of flow in porous media is undergoing a renaissance, invigorated by new applications and challenges, and powered by a range of novel numerical, analytical, and experimental techniques (2).

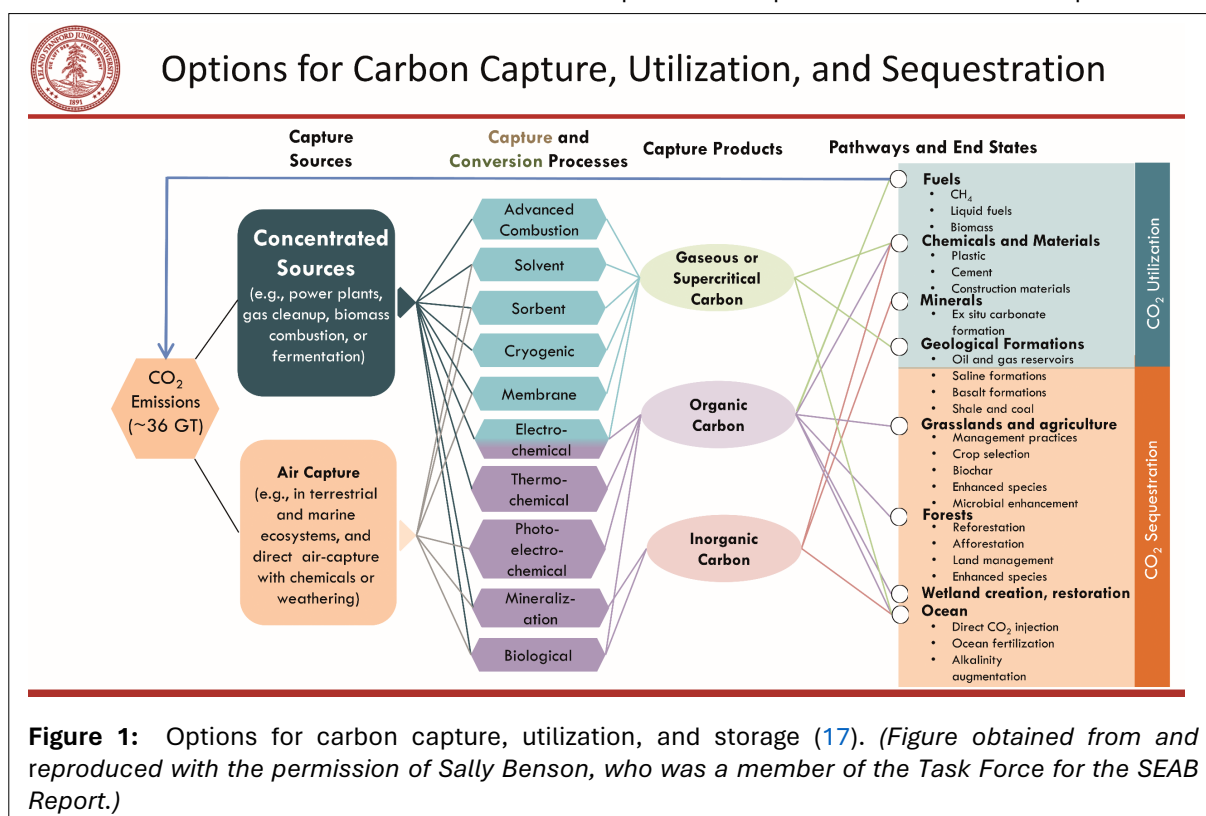
2. CARBON DIOXIDE STORAGE

Fifty years of CO₂ injection for enhanced oil recovery has provided abundant evidence that CO₂ can be handled safely and retained indefinitely in the subsurface if sites are carefully evaluated and chosen, and the projects are designed, operated, and monitored appropriately (1, 8). While CO₂ can be stored in depleted oil and gas reservoirs, storage in deep saline aquifers is needed to take advantage of the worldwide distribution of porous sedimentary rocks with structural traps and low-permeability formations above the storage zone that prevent early vertical migration of CO₂. Considerable research effort (including that presented at the InterPore Conference) has been devoted to quantifying the physical mechanisms that describe flow during the injection phase in heterogeneous formations and trap the CO₂ on longer time scales. These include capillary trapping of residual CO₂ bubbles surrounded by water, dissolution of CO₂ in the brine (which removes the driving force for upward vertical migration of CO₂), Ostwald ripening of larger CO₂ bubbles at the expense of smaller ones (see below), and mineralization reactions that convert CO₂ to solid carbonate minerals.

Based on this experience, CCS can be deployed at a much larger scale than it is today, although some combination of incentives, a price on emissions of CO₂, or regulatory limitations on emissions will likely be required for that to happen at a gigatonne scale (13). In addition, CCS will have to compete with other options for the mitigation of emissions, and thus, the cost matters. The largest cost element in any CCS project is the capture of CO₂, typically from combustion products or other process gases. The separations area is rich with research questions that involve porous media, often in combination with designed sorbents, engineered micro-structured materials and coatings, membranes, and reactions mediated by electrochemistry, thermochemistry, photochemistry, or phase changes (see Fig. 1 for a catalogue of capture and storage options).

Extensions in the range of subsurface storage formations would provide more possibilities for storage in locations with limited access to more conventional settings. Basalt formations have been considered, but there is much more to be done to explore the effects of carbonate mineral precipitation on permeability, modification of fracture flow paths, and the kinetics of mineralization reactions that are expected to occur. Storage in sediments below the seafloor, where temperatures are low enough for hydrates to form, could offer potential storage offshore, although many questions regarding flow management and long-term stability remain (4). Some mine tailings contain sufficient reactive minerals to create the possibility of storage at surface sites. Storage based on adsorption in shales and deep coal seams, presumably fractured to accommodate reasonable flow rates, could provide suitable locations; if required seals are present, pressures can be managed, and drilling costs can be controlled. Only limited work has been conducted on these cases.

Further research is required to evaluate the factors influencing the long-term security of CO₂ stored in saline aquifers, particularly for the volumes that remain in the free phase. There are pressure gradients across most large aquifers that cause hydrodynamic flow. Changing or unexpected aquifer flows may result in CO₂ spilling from apparently secure structural traps. This could be because they are connected to the surface (e.g., the Alberta Basin aquifer is recharged by rainfall in the Rockies) or the seafloor (e.g., the Bunter Formation that will be used in the Endurance storage project) (19). Alternatively, pressure gradients can be caused by geological processes that occur over thousands to millions of years, such as glacial unloading, hydrocarbon generation, or differential compaction. There is a need to develop methods to better characterize communication in open saline aquifers, both across the aquifer and to



the seafloor or Earth's surface. Human activity can also cause flow due to hydrocarbon production or extraction of potable water for drinking or irrigation. In the future, if climate change is not halted, these pressure regimes could change because of increasing sea levels, changing rainfall, increasing glacial unloading, or the melting of hydrate seals. We know that when hydrocarbons migrate from source rocks, a proportion are trapped, and the remainder ultimately escapes to the surface. Estimates suggest that 0.6Mt/yr of oil (12) and 40Mt/yr of methane (16) are naturally seeping to the surface each year. Although these are small quantities compared with the masses of hydrocarbons in place and the masses of CO₂ that will be stored each year (Gt), over millennia, the total mass leaked becomes significant.

Considerable progress has been made in modeling the multi-spatial-scale, multi-time-scale, and multi-mechanism flows that occur in the subsurface storage of CO₂. More work is required to fully integrate thermal and geomechanical effects as well as long-term geological processes. Pressure management and avoidance of fault activation and induced seismicity will be important, especially for social acceptance of storage projects. Protocols for evaluating long-term security need to be developed, perhaps based on those used to evaluate sites that will be used for permanent storage of nuclear waste. Full physics models have great utility as a tool for designing injection processes that accelerate the immobilization of CO₂ through combinations of trapping mechanisms and these models help to identify which physical mechanisms are most important in a specific setting. Deployment at scale would also be aided by the availability of more limited (and easier to use) models that focus on the most important transport mechanisms for the systematic characterization of storage formations and sites. The development of characterization protocols that allow early and then steadily more refined estimates of reservoir capacity, permeability, seal integrity, areal extent of CO₂ migration, and maximum pressure rise would streamline project development, considering that gigatonne-scale storage will require thousands of projects worldwide. In addition, the development of efficient and low-cost monitoring protocols appropriate to the type of storage formation would provide a framework for safe and effective operation. This involves anticipating and managing risks such as leakage out of the zone, loss of seal or well integrity, excessive pressure rise, or adverse effects of long-term geological processes. A well-designed emergency response plan consistent with the risk analysis is also essential. These elements should be part of a systems approach for capturing CO₂ from multiple industrial and power generation facilities, transporting the CO₂ to storage sites, and carefully engineering and operating subsurface storage operations. Public acceptance of CCS on a large scale requires early and open communication about the measures being taken to protect the public and workers during both the injection and post-closure phases of a storage project.

3. COMPRESSED GAS AND HYDROGEN STORAGE

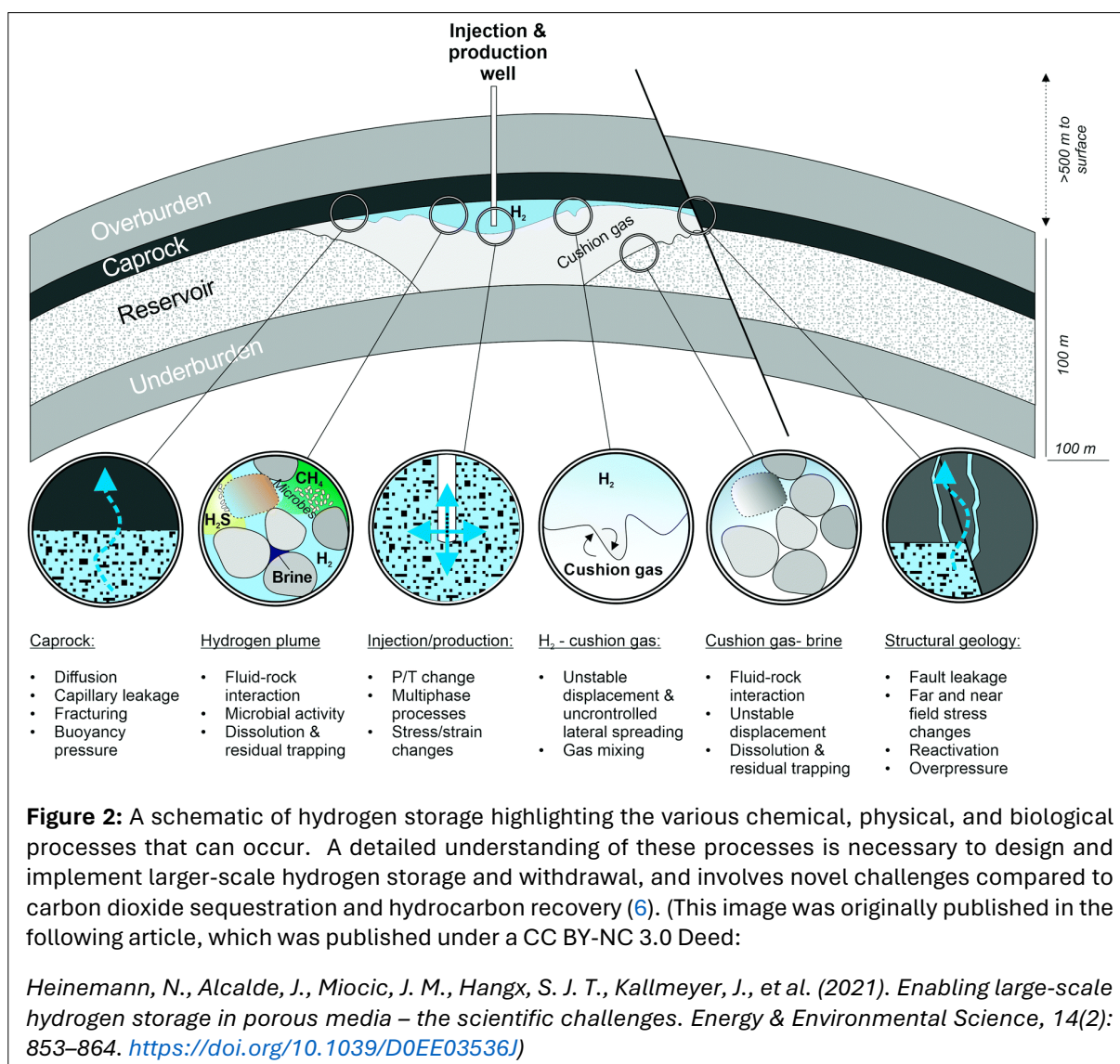
Energy can be stored in three ways – as thermal energy (discussed in the next section), through pressurizing a gas, or from combustion. To place some numbers in context, the thermal energy released when 1 kg of water changes temperature by 100 K is approximately 0.42 MJ. This is almost exactly the same as the pressure-volume work released from 1 kg of nitrogen (molecular mass, $m = 0.028$ kg/mol) changing pressure from $P_1 = 10$ MPa to $P_2 = 0.1$ MPa (100 to 1 bar) at ambient temperature ($T = 288$ K), $E = \frac{RT}{m} \ln \left(\frac{P_1}{P_2} \right) \approx 0.41$ MJ. However, much more energy can be stored through the heat of combustion which is highest – on a mass basis – for hydrogen when compared to any other gas at 120 MJ/kg.

Global energy use is approximately 640 EJ per year, or around 20 TW (14), so worldwide storage is required at the gigatonne scale to store energy over long seasonal periods. If we consider the storage of, for instance, 100 EJ (10^{20} J) globally, this is equivalent to 200 Gt of water or compressed gas, using the assumptions above, or 1 Gt of hydrogen. As with carbon dioxide, this capacity is only available in subsurface porous reservoirs. We will discuss thermal energy storage in the next section. For hydrogen storage, the technology is less well established than for carbon dioxide sequestration; most underground storage of hydrogen to date has been in engineered salt caverns. Salt caverns have a greater capacity

than above-ground facilities but can only be made in specific regions where thick salt layers are present underground. In contrast, porous reservoirs are more abundant in sedimentary basins.

Figure 2 illustrates the physical, chemical, and biological processes that occur during hydrogen storage in porous reservoirs (6). The major difference between hydrogen storage and carbon dioxide sequestration is that hydrogen must be both injected and withdrawn, usually on a seasonal cycle. Hence, mechanisms such as dissolution and reaction, which are favorable for carbon dioxide, as mentioned above, ensuring its long-term retention in the subsurface, are detrimental to hydrogen as they represent a loss of a valuable energy store.

The first process that needs to be studied is the hysteresis effect due to repeated cycles of injection and withdrawal. Traditionally, in hydrocarbon systems, only a single cycle of primary drainage (initial accumulation in the field) and water or gas flooding need to be considered; however, we need to determine the averaged relative permeability and capillary pressure characteristics for arbitrary cycles of drainage (hydrogen injection) and imbibition (hydrogen production). Furthermore, although hydrogen is only partially soluble in reservoir brines, transport of dissolved hydrogen through the aqueous phase can be significant. Specifically, a process called Ostwald ripening can occur from the pore-to-field scales (7): local differences in capillary pressure between ganglia of the gas phase lead – through Henry's law – to slight differences in solubility, establishing concentration gradients in the aqueous phase. Through molecular diffusion, hydrogen diffuses more quickly than heavier gases, leading to the transport of



hydrogen from regions of high to low capillary pressure. Eventually, capillary pressure equilibrium is reached through the rearrangement of the gas phase in the pore space. The time scales and impact of this process, which is negligible in oil/brine systems, need to be studied and its impact on field-scale storage assessed. It is possible that existing hysteresis models based on oil-water flow need to be updated.

In both porous reservoirs and salt caverns, hydrogen is stored above a cushion gas, which maintains the pressure and limits the trapping of hydrogen by water. This gas could be initially present in the reservoir, such as methane, if storage occurs in a depleted gas field, or injected if we consider nitrogen or carbon dioxide. The mixing of hydrogen with cushion gas, facilitated by the high diffusion coefficient of hydrogen combined with the flow from injection and withdrawal, could result in the production of both hydrogen and cushion gas, which would need to be separated at the surface, adding to the cost of storage. Again, this process must be studied carefully for a range of flow conditions.

The hydrogen can also interact with the cap rock in a storage formation, or with the salt lining of a cavern. In addition, it is known to diffuse into metal components, causing embrittlement. The effects of hydrogen interactions with both engineered and natural components of the storage site are further areas of research, as well as the design of hydrogen-resistant materials.

During injection, the reservoir pressure will increase and decrease during production. This repeated change in the stress state results in mechanical hysteresis and changes in the pore structure and permeability. The long-term impact of pressure changes and the possibility of weakening the formation or inducing fracturing are other active areas of study.

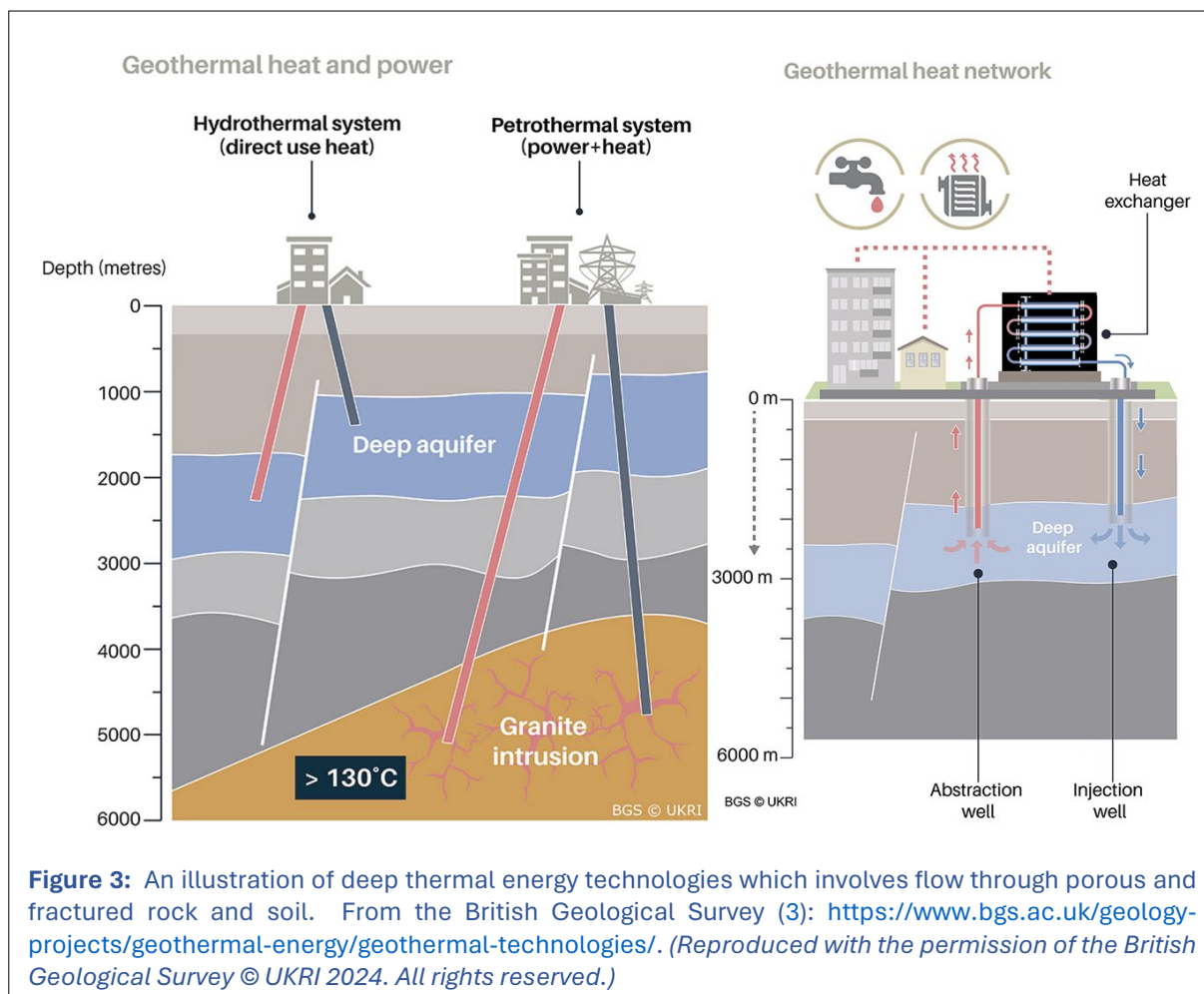
Finally, and most importantly, is the impact of chemical and biological processes. Hydrogen can react with iron-containing minerals that are often present in sandstone. More significant, and a key uncertainty in the assessment of hydrogen storage, is the presence of bacteria that can degrade hydrogen, particularly in the presence of other foods, such as hydrocarbons. The extent of bacterial activity depends on the salinity and temperature conditions, being suppressed in highly saline environments and at temperatures exceeding 100°C. Bacterial activity often results in the formation of H₂S, which is toxic and must be removed from the produced gas stream. A hydrogen storage project is only viable if bacterial degradation is minimal; unfortunately, in some of the few field sites where mixtures of hydrogen and methane have been stored, degradation was significant (7).

If hydrogen plays a significant role as an energy storage and carrier, gigatonne (exajoule)-scale storage is required globally. This can only be supplied in underground porous reservoirs – either aquifers or depleted natural gas fields. Site assessment is crucial, with the principal concern being the mixing of cushion gas and bacterial degradation. Further research from the laboratory to the field is required to understand and design efficient storage systems.

4. GEOTHERMAL ENERGY AND THERMAL ENERGY STORAGE

The interior of the earth is hot, thanks to its high temperature from planetary formation and radioactive decay. Warm water from underground, particularly near tectonic plate boundaries, where hot rock is encountered close to the surface, has been used for heating since before Roman times.

The potential resource is huge; the thermal energy of the whole planet is 10³¹ J, which is more than sufficient to meet the world's energy needs sustainably (11). The most recent assessment estimated up to 108 GW of installed thermal energy in 88 countries worldwide, growing at a rate of 8.8% per year (11). There are two distinct types of geothermal resources. The first exploits the extraction of very hot water from the deep subsurface (below 500 m), as shown in **Figure 3**, often at steam temperatures to generate electricity or to be used directly for heating. Deep geothermal energy is only economically viable at present in limited parts of the world, including the US, Iceland, El Salvador, Kenya, the Philippines, and New Zealand, because the hot rock must be sufficiently close to the surface to allow drilling and fluid extraction. The second and potentially more significant resource is simply to make use of soil and water



just below the surface, which maintains an almost constant temperature throughout the year. This resource can be exploited for heating and cooling. This is significant, as in many parts of the world, up to 50% of the total energy is consumed for space heating and cooling using fossil fuels (3). Ground-source heat pumps can be used for shallow resources to provide warm water throughout the year. Furthermore, groundwater can be used to store thermal energy. In ATEs – aquifer thermal energy storage – for instance, cold water can be extracted for cooling in summer and then re-injected as warm water in an adjoining well. During winter, this warm water is pumped out for heating and cooler water is re-injected into the cold water zone. This is a nascent technology in terms of global implementation, but it is already well established in the Netherlands (5).

These two types of energy sources are associated with distinct research challenges. For geothermal energy, water is generally extracted from hot fractured rock. Here, the research challenges are the understanding of the complex fracture network in the deep subsurface, fluid flow, and the phase change between steam and hot water. Additionally, the development of efficient drilling and potential fracturing technologies for deep igneous rock is important. Another area of research is the management of the fluid used to extract heat, which is normally water, either originally present in the formation or injected and cycled. However, there is growing interest in the application of supercritical CO₂, for instance, that has a low viscosity and reasonably high heat capacity, and offers an attractive alternative with the advantage that any fluid loss contributes to carbon storage.

For aquifer thermal energy storage, the main challenges are understanding the dispersion and movement of the thermal plume in a heterogeneous subsurface and optimizing the storage and conversion efficiency. Unlike large-scale projects associated with the oil industry and carbon dioxide storage, the use of shallow groundwater for heating and cooling is smaller-scale and usually used for

small districts or single large buildings; therefore, there is less time and money available for individual site assessments. Other avenues for research include chemical and biological activity: altering the subsurface temperature will affect the local ecosystem, with a potential impact on drinking water supplies, as well as causing problems associated with bacterial fouling. Unlike hydrogen storage, these problems cannot be overcome by operating in sterile environments.

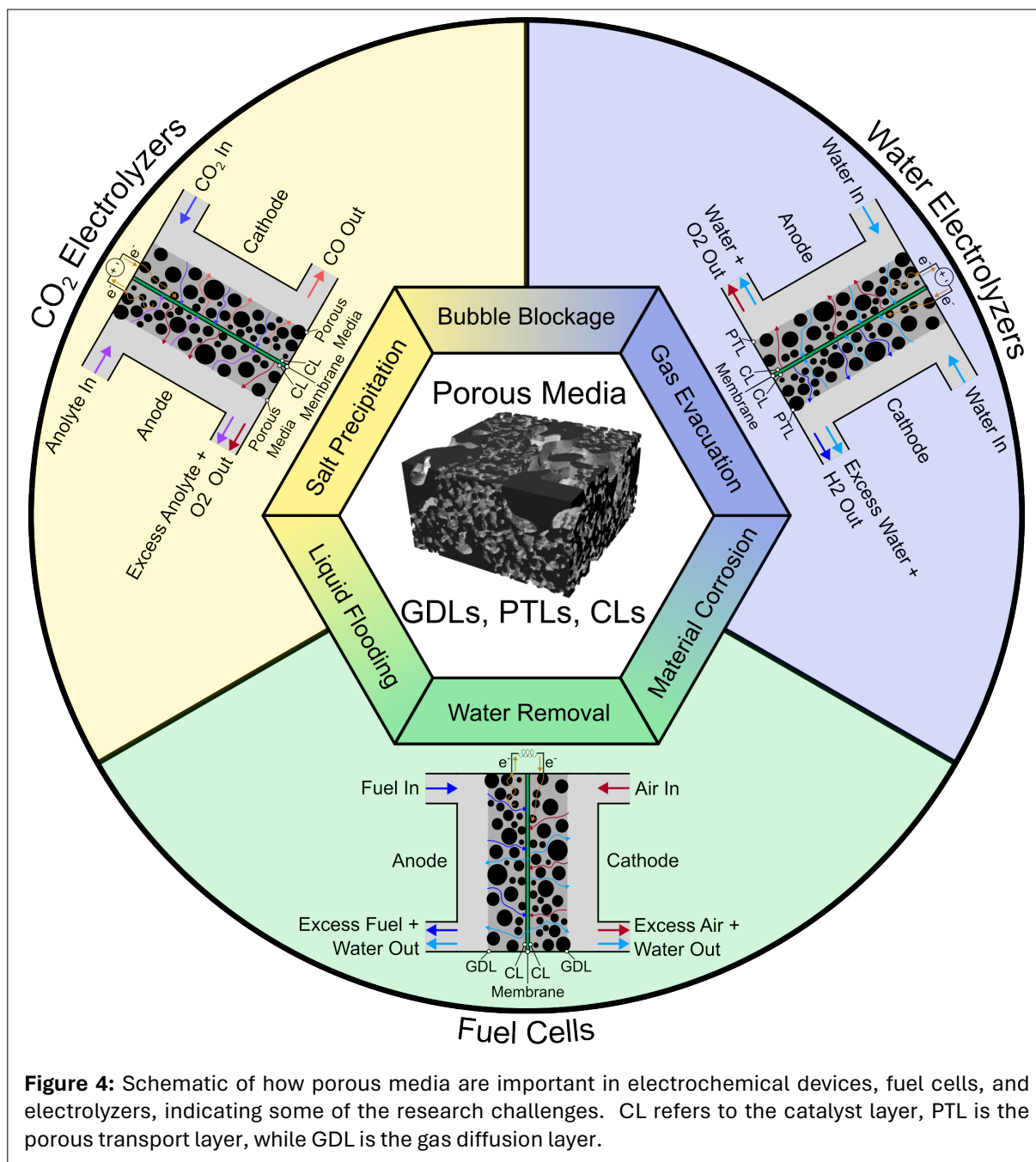
Overall, the rapid increase in geothermal energy use, albeit from a small base, offers a significant potential contribution to efforts to meet net zero, particularly by providing a sustainable low-carbon resource for space heating and cooling. The porous media community has an important role to play in site characterization and in understanding coupled chemical, mechanical, biological, and flow processes in geothermal and heat storage projects.

5. ELECTROCHEMICAL DEVICES

Shifting away from fossil fuels is not the only step needed to achieve a sustainable future; we must also change the way we convert energy from one form to another. Electrochemical energy conversion is a class of technologies that converts one form of energy into another electrochemically (i.e., in the absence of combustion). This field includes fuel cells and electrolyzers, whose performance relies crucially on multiphase flow through porous materials at different length scales, as illustrated in [Figure 4](#). Hydrogen fuel cells convert hydrogen and oxygen from air into electricity and heat, respectively. Conversely, water electrolyzers split water into hydrogen and oxygen but require a power source (9). Over the last few years, carbon dioxide electrolysis has emerged as a promising technology for electrochemically converting carbon dioxide into useful chemical feedstocks and carbon-neutral fuels (15). Once thought to be far too power hungry to ever be practical, CO₂ electrolyzers are receiving a growing level of attention as technology advances rapidly. While each of these technologies has a different purpose – producing electricity, producing hydrogen, or sequestering CO₂ into carbon neutral fuels or chemical feedstocks – what they share are architectures that generally involve polymer membranes (or liquid electrolytes) paired with porous transport media and flow fields. Critically, these technologies must achieve effective electrical, heat, and mass transport to be efficient, durable, and cost-effective.

While there are a variety of fuel cells, the low-temperature polymer electrolyte membrane fuel cell is one of the strongest contenders for impacting the energy transition because it is most suitable for transport applications, from light duty to heavy-duty vehicles, as well as buses and trains. They operate below 100°C, which is ideal from a heat management perspective, where consumers and operators are the general public. However, in this low temperature range, liquid water is prevalent.

In fuel cells, we need water to hydrate the polymer membrane to provide ionic conductivity, and when hydrogen and oxygen are combined, liquid water is the product. While water itself is not harmful, the liquid tends to saturate the porous materials that are needed for gaseous reactant delivery within the fuel cell itself. The gas diffusion layer (GDL) is a porous carbon textile that is on the order of 100-200 μm thick and is made of carbon fibers approximately 10 μm in diameter, forming a layer with pores ranging from 30-100 μm across. These materials are typically rendered hydrophobic through partial coating with a plastic (usually PTFE) binder to encourage water evacuation; however, these materials typically exhibit mixed wettability conditions. Their irregular pores and mixed wettability lead to highly complex liquid water saturation patterns and residual saturations. Furthermore, wettability treatments have been shown to degrade over time, further complicating efforts to control the water management. To help mitigate water management problems and reduce ohmic losses, an additional nanostructured coating, termed the microporous layer (MPL), can be applied to the GDL. However, exactly how to design the MPL structure (with or without cracks), how thick it should be, and how far it should be embedded into the GDL (or extend from it) are all parameters that are not well correlated with performance. While there are major strides in the field of fuel cells to reduce precious metal use for cost-effective catalyst layers, the optimization of the gas diffusion layer and the interfacial conditions between the gas diffusion layer and the catalyst layer remain a key focus for which expertise in porous media is required.



The field of electrolysis has an advantage over fuel cells. First, it can leverage the work that has already been done in fuel cells. Second, water electrolyzers have already been commercially deployed because of their need in other industries such as industrial processing and nuclear power. However, to meet the cost and durability targets needed for the energy transition (such as that laid out by the US Department of Energy), water electrolyzers have a long way to go. In terms of durability, they need to go from 40,000 to 80,000 hours lifetime, while providing hydrogen with an estimated overall cost (including power generation) of less than \$1 per kg – just two examples of the major improvements that are needed (18). At the pore level, water electrolyzers must also contain a porous material with a function similar to that of the fuel-cell GDL. However, in most devices, this is a titanium porous transport layer (PTL). Titanium, although expensive, is the main option for withstanding the highly corrosive environment of the electrolyzer. The PTL is typically composed of sintered titanium particles or a titanium fibrous mesh. Rather than requiring the PTL to be devoid of product water, the PTL must be fully saturated with liquid water at the anode so that the reactant can be delivered as efficiently as possible to the anode catalyst layer. Furthermore, air or oxygen bubbles can create hotspots that may lead to material damage.

Rendering a super-hydrophilic material is an approach, but it does not solve the problem entirely because oxygen gas is continually being produced within the water electrolyzer and requires a high capillary pressure to escape the system. These gas bubbles must flow in the opposite direction to the incoming reactant water; however, this competing flow is a major bottleneck for achieving ideal mass transport conditions. Designing the PTL for oxygen bubble transport is key, but there are a variety of questions on how to advance the water electrolyzer PTLs, including what is the ideal thickness, what is the ideal interface with the catalyst layer, and what should the pore shape be (10).

The CO₂ electrolyzer is in its infancy, particularly when compared to the other technologies described in this section. There is a tremendous opportunity to leverage the knowledge curated within the fields of fuel cells and water electrolyzers. However, there are also some notable differences. A variety of architectures are being explored, and this creative landscape may offer unique opportunities, such as H-cells, flow cells, and membrane electrode assemblies (MEAs). Even within the MEA category, various membrane configurations are possible, and each will require a different architectural setup. Making each of these architectures viable will involve the careful management of CO₂ reactant, electrolytes, products, and the porous media. Flow channels must be selected to enable these transport processes effectively.

Overall, the application of flow and transport skills in porous media offers the opportunity to develop cheaper, more robust, and more efficient electrochemical devices that will play a vital role in the energy transition.

6. SOCIETAL ENGAGEMENT

The energy transition is a major societal concern with a significant impact on everyone's lives, from the effects of climate change, the economic costs of changes and disruptions in energy supplies, and the major infrastructure involved in large-scale power generation by renewables combined with subsurface storage.

It is already apparent from public discussions on the siting of wind farms, carbon dioxide storage, and geothermal energy, for instance, that having a technology that is viable from an engineering and financial perspective is not sufficient for its implementation. The regulatory framework must allow major developments to occur, and the public, particularly those most likely to be affected by energy projects, must be involved in decision-making. Concerns about induced seismicity and leakage from storage sites, for instance, need to be addressed seriously, appreciating concerns from the perspective of the population where renewable energy or storage sites are planned.

Scientists must engage with the wider public to help facilitate an effective transition to a zero-carbon economy. This involves the provision of expert and unbiased information in areas of expertise while listening to and appreciating wider concerns regarding new technologies.

7. CONCLUSIONS

This document highlights some of the research challenges involving porous media that are relevant for the energy transition. The success of InterPore as a society, with the vibrant and stimulating atmosphere at the 2023 Annual Meeting in Edinburgh, attests to the vitality of the subject. The discipline of flow in porous media is undergoing a renaissance. We trust that this document helps frame important research questions and stimulates further development in this exciting and growing field.

STATEMENTS AND DECLARATIONS



Author Contributions

All authors contributed to the preparation of this article, including the drafting, revising, author corrections, and final approval.

Conflicts of Interest

There are no conflicts of interest to declare.

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