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*Review*

# Multiple microorganism influences and interactions limit the reliability of underground hydrogen and carbon storage simulation models at the reservoir scale

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**Abstract:** The various types of microorganisms encountered in subsurface reservoirs are identified, and their consequences for underground hydrogen storage and carbon dioxide storage are described. In underground hydrogen storage reservoirs, most microorganism activities have negative consequences (pore clogging, reduction in permeability, corrosion, change in composition and loss of stored gas). In underground carbon dioxide storage most of those negative consequences also apply, but transforming some of the stored $CO_2$ into methane by the biomethanation process can be beneficial and potentially exploited. Although laboratory studies and simplified-system simulations have qualitatively explained the microorganism processes involved at the pore scale in underground hydrogen storage and underground carbon dioxide storage reservoirs, it is difficult to model these processes quantitatively at the reservoir scale. The simplifying assumptions, scales and dimensions of the majority of bioreactive transport models fail to take adequate account of reservoir heterogeneities, biofilm development complexities, periodic fluctuations in fluid-flow and nutrient supply. These limitations mean that most of the existing bioreactive transport models are unable to reliably quantify changes in gas composition, gas loss, permeability, or the degree of corrosion likely to occur across heterogeneous underground hydrogen storage or underground carbon dioxide storage reservoirs. However, several opportunities exist to improve field-scale bioreactive transport model performance for underground hydrogen storage and underground carbon dioxide storage in the coming years. These include building on the knowledge gained from the existing simplified models by incorporating new modelling techniques and more detailed reservoir scale information. Exploiting DNA sequencing offers the capability to better characterize the properties of reservoir microorganism communities. Physics-informed machine learning techniques could be tailored to provide efficient surrogate models for simulations of heterogeneous reservoirs. Such improvements should lead to simulation models capable of accommodating more complex reservoir-scale assumptions.

**Keywords:** Microorganism $H_2/CO_2$ transformations; gas storage reservoir heterogeneities; bioreactive transport complexities; biofilm characteristics; biomethanation

## 1. Introduction

In recent years, underground hydrogen ($H_2$) storage (UHS) has emerged as the primary feasible option for storing large quantities of $H_2$ for short- and medium-term periods (Hassan et al., 2021; Sekar et al., 2023; Bosu and Rajamohan, 2024; Davoodi et al., 2025). However, this technology has to overcome multiple environmental and operational challenges, including risks of leakage and performance degradation due to microorganism activities (Wood, 2025). Exploitation of subsurface carbon storage and utilization in the form of enhanced oil recovery (EOR)

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has also expanded substantially in recent years (Liu et al., 2023a; Davoodi et al., 2023; 2024).

In well-sealed underground gas storage for natural gas (UGS), $H_2$ (UHS), and $CO_2$ (UCS) reservoirs, the loss of gas through abiotic processes over the medium term tends to be very low. However, biotic processes associated with microorganism (archaea and bacteria) activities can lead to substantial gas loss and redistribution, particularly in the case of $H_2$ (Hassanpouryouzband et al., 2022). In particular, pore clogging by biofilms can substantially impair permeability, consume stored $H_2$, and alter fluid flow channels, potentially impeding injectivity and productivity. The spectrum of adverse UHS outcomes that can be caused by microorganism activities is summarized in Fig. 1.

The term biofilm refers to structured communities of microorganism cells which may develop into a larger/thicker accumulation sometimes referred to as a biomat; in this study, the term biofilm is used to refer to both biofilm and biomat structures. Sekar et al. (2023) described the various ways in which microorganism activities interact with the fluid dynamics in UHS.

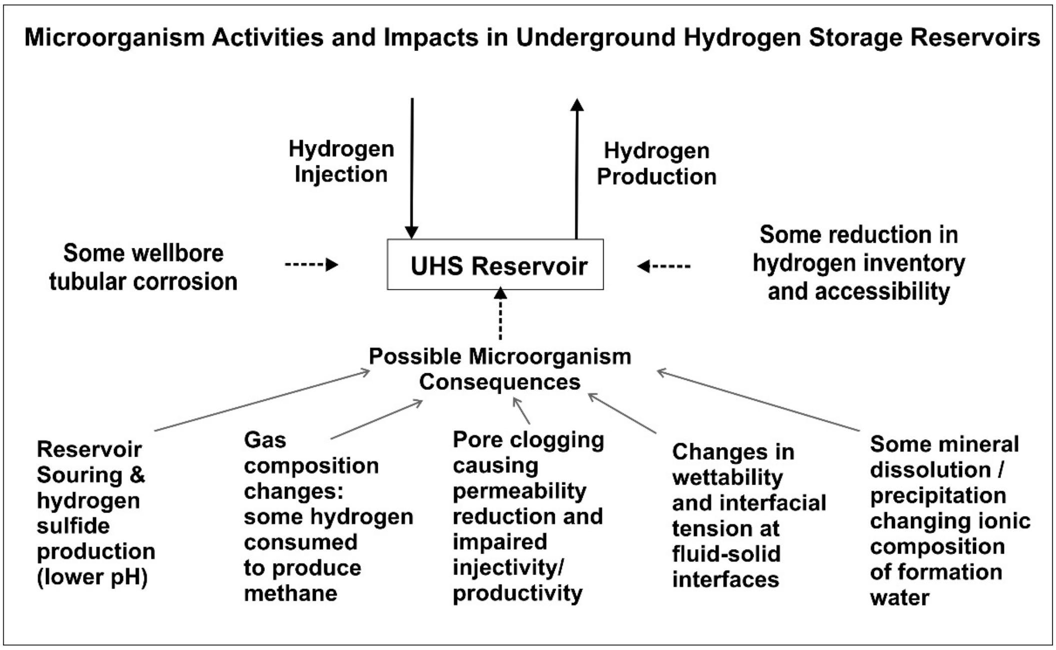

**Fig. 1.** Microorganism activities and impacts that can potentially occur in UHS reservoirs.

Reservoir heterogeneity involves spatially variable porosity and permeability, which leads to variable fluid-flow rates throughout the reservoir. Microorganisms' metabolic rates vary with prevailing fluid-flow rates because those rates influence the rates at which nutrients are provided to the microorganisms. Biofilm complexity involves variable thickness, porosity, and permeability throughout a biofilm, and this influences the flow rates at which nutrients are delivered to individual cells within the biofilm. Hence, different parts of a biofilm may develop at different metabolic rates due to differences in their nutrient supply. Consequently, reservoir simulation models that assume homogeneous (constant) reservoir and biofilm porosities and permeabilities lead to erroneous predictions regarding reservoir-wide microorganism metabolism and $H_2$ consumption rates in heterogeneous reservoirs.

## 2. Subsurface microorganism communities and processes

### *2.1 Distinct groups of subsurface microorganisms*

There is a plethora of microorganism species that exist in the Earth's upper crust that have evolved in various ways to exploit hydrocarbons, $H_2$, and $CO_2$ in the subsurface as energy sources. Extensive work on improved and enhanced oil recovery processes has illustrated the diversity of microorganisms and the ability of different species to function in aerobic, anaerobic, and facultative (with or without oxygen) conditions to the benefit or detriment of subsurface reservoir properties (Wood, 2021). $H_2$ has been produced in the Earth's crust and recycled through it via sea floor sediments and the mantle for billions of years (Wood, 2025). This has enabled microorganisms to evolve to exploit it in various and sophisticated ways as it passes through the crust. Indeed, few reservoirs of naturally occurring $H_2$ can survive for long periods in the upper crust without ultimately being degraded by $H_2$-consuming microorganisms (Wood, 2024).

Experiments and simulations have demonstrated that the biodiversity of microorganism species and their lifestyles can substantially impact UHS efficiency. Safari et al. (2025) highlighted six different groups of microorganisms and their different impacts on UHS efficiency at depths~1600 m (~60 °C) (Fig. 2). Some species in those groups have the ability to survive at substantially higher temperatures. The coexistence of multiple microorganism groups in UHS reservoirs influences the rate at which $H_2$ is consumed because each species in each group has a distinct metabolism. Hence, each species consumes $H_2$ at different rates. The metabolic rate of each species also

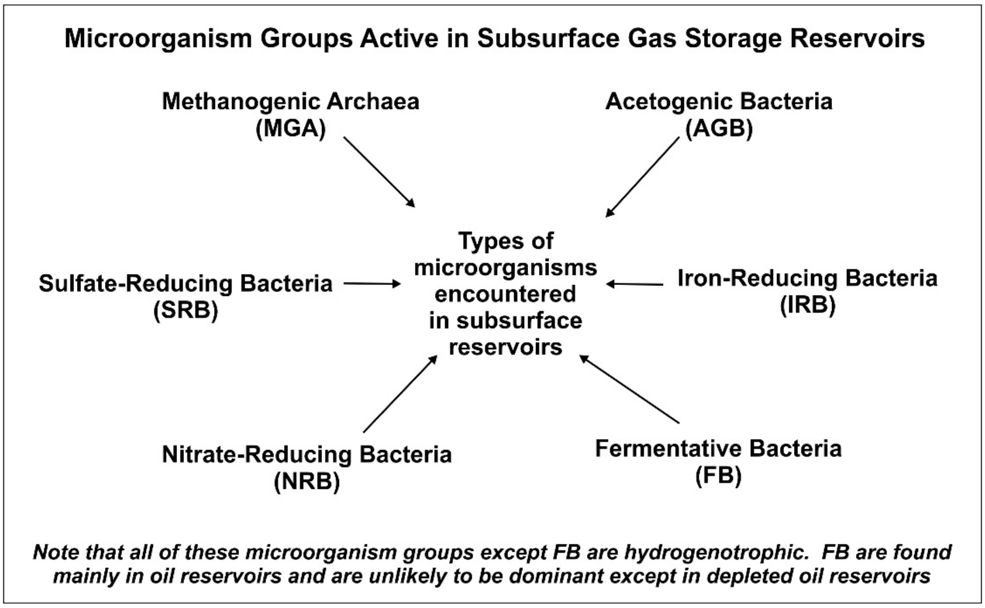

**Fig. 2.** Six groups of microorganisms potentially active in UHS reservoirs. Information adapted from Thaysen et al. (2023) and Safari et al. (2025).

changes with changes in reservoir temperature and with electron acceptor availability. Moreover, the potential for coexistence of some of these groups in UHS facilities and their impacts on microorganism community kinetics and fluid movements at reservoir scales is not yet fully established or understood.

Microorganism communities typically consist of groups of individual cells, each surrounded by extracellular polymeric substances (EPS), which together constitute a biofilm. The positions of biofilms within a reservoir formation, typically at gas-liquid interfaces or fluid-solid interfaces (pore walls), determine their structure and development (Imani et al., 2026). The more motile biofilms existing at fluid-fluid interfaces are less understood than the more static ones developed at fluid-solid interfaces. Adhesion between the cells of planktonic microorganisms, as well as their hydrophobic tendencies, influence biofilm formation at fluid-fluid interfaces (Subbiahdoss et al., 2020). Microorganism community activities have multiple flow-dynamic influences on UHS systems depending on their growth conditions (Dopfell et al., 2021). Certain conditions can exacerbate the risk of adverse consequences, such as $H_2$-flow inhibition by pore clogging and metallic corrosion (Thaysen et al., 2021).

Four of the micro-organism groups distinguished in Figure 1 are hydrogenotrophic, meaning that they exploit $H_2$ as an energy source. Hydrogenotrophic methanogenesis is the process by which methanogenic microorganisms convert hydrogen ($H_2$) into methane ($CH_4$). It is an anaerobic process in which $H_2$ combines with carbon dioxide ($CO_2$) to generate and water ($H_2O$) to form $CH_4$. In UHS and UCS reservoir formations, this process tends to become concentrated at the interfaces between gas and liquid and fluid and solid. Microorganism activity at these interfaces leads to physicochemical changes in interfacial tension (IFT), wettability (quantified by contact angle (CA; $\theta$) measurements), and capillarity (interactions between surface tension and adhesion in the case of fluid-solid interfaces). These changes tend to promote gas bubble disconnection and accelerate the methanogenetic reactions.

Hydrogenotrophs are microorganisms that exploit $H_2$ as an electron donor. Some do this to convert $CO_2$ into $CH_4$, or acetate ($CH_3COO^-$), or other hydrocarbon compounds. Sulfate-reducing hydrogenotrophs, mainly sulfate-reducing bacteria (SRB), exploit sulfate as an electron receptor to generate hydrogen sulfide ($H_2S$; a toxic and corrosive gas). Alternative metabolic types are: acetotrophs (splitting $CH_3COO^-$ into $CH_4$ and $CO_2$); methylotrophs (transforming methanol and methylamines into $CH_4$); syntrophic bacteria (oxidizing fatty acids into $H_2$). Hydrogenotrophs, acetotrophs, and methylotrophs can, in theory, function simultaneously in methanogenesis. The highest temperatures at which methanogenic microorganisms have been observed experimentally to survive are 122 °C at high pressure (Takai et al., 2008).

$H_2$ in most subsurface reservoirs would naturally be impacted by hydrogenotrophic reactions associated with microorganism assemblages and their various metabolisms. Key reactions encountered are biomethanation generated by the Sabatier reaction, producing $CH_4$ from $H_2$ and $CO_2$, sulfate-reduction, and iron-reduction reaction. The impacts of such reactions have been modelled from a hydrodynamic perspective, making certain simplifying assumptions (e.g., Hagemann et al. (2016)).

The mentioned microorganism groups (Fig. 1) tend to flourish in different environmental conditions, so microorganism communities tend to be dominated by certain groups in specific reservoir locations. In Fe-rich and sulfate-rich locations, iron-reducing (IRM) and sulfate-reducing (SRM) methanogens, respectively, can outperform the other groups as they require less energy to achieve their molecular transformations. This also means that IRM and SRM may be able to flourish in the $H_2$-poor regions of biofilms more than other microorganisms. IRM also includes dissimilarity iron-reducing bacteria (DIRB) types that act with $H_2$ to reduce $Fe^{3+}$ to $Fe^{2+}$ in anoxic conditions (Zhao et al., 2025). Methanogenesis, therefore, tends to be dominant, compared to SRM and IRM, when there are relatively few electron receptors.

The presence of sulfide ions in saline formation water substantially influences $H_2S$ concentrations in the reservoir fluids. $H_2S$ serves as a nutrient for sulfate-reducing microorganisms (SRM), which can exist natively in a formation, or be introduced deliberately or inadvertently (e.g., during drilling or UHS/UCS operations). Further studies are needed to quantify the amount of $H_2S$ generated under different reservoir conditions and to propose mitigation measures to keep operations safe.

As well as a hydrogen supply, each of the mentioned microorganism groups requires additional nutrients (particularly N, P, and S), plus small quantities of certain metals (e.g., Fe and Mn) and vitamins (Thaysen et al., 2021).

### *2.2 Linking DNA data to microorganism activities*

It is now possible to characterize UHS/UCS microorganism communities applying DNA sequencing techniques, specifically metabarcoding and metagenomics (Pinto and Bhatt, 2024). Belcour et al. (2025) have developed a method to derive high-level biogeochemical cycle estimates from metabarcoding data, which can be used to distinguish the main metabolic functions of a reservoir microorganism community (e.g., hydrogen oxidation, sulfur reduction, and/or carbon fixation). They tested the method with datasets from two salt-cavern storage facilities and were able to verify its estimates of microorganism activity and water compositions for data from those facilities. Such information can be used to predict the type of $H_2$ consumption most likely to occur at specific reservoir locations and the gas compositional changes that are likely to result from that activity, That study was conducted as part of the “Hylife” initiative of researchers from four European countries to determine microbial risks associated with hydrogen underground storage in Europe (www.hylife-cetp.com (accessed on 20 December 2025)).

There is considerable and variable potential for microorganism $H_2$ consumption in UHS reservoirs. This introduces uncertainty regarding the stability, safety, and long-term integrity of these facilities as gas storage repositories. A key reason for the variability is the wide range of conditions and microorganism communities that exist in these reservoirs and can potentially flourish as $H_2$ is injected into them. Cerna et al. (2025) have provisionally developed and tested in multiple laboratories a reservoir brine testing and analysis procedure. It determines $H_2$ consumption by microorganisms, the composition of the resulting gas, and brine pH. The value of such an approach is that it can be used to quantitatively assess specific UHS reservoir candidates for their microbial $H_2$ consumption rates and compare those rates with standards. Access to such information removes some of the uncertainty regarding microorganism consumption rates at specific reservoir locations. It also enables some of the biotic growth kinetic terms of reservoir models to be suitably tailored to specific reservoir conditions. Potential exists to link such standardized testing to metabarcoding data and expand the characterization to include microorganism community DNA information for a wide range of subsurface reservoirs.

### *2.3 Microorganism and biofilm cell growth*

Microorganism growth is driven by environmental conditions, with nutrient availability, pH, pressure, salinity and pressure exerting the most influence (Ahn et al., 2022). Their lifestyles typically develop and evolve through a distinct sequence of steps (Fig. 3). Extreme UHS reservoir environmental conditions tend to limit microorganism viability and also impact biofilm growth, texture (e.g., pore space), and displacement kinetics. The preferred lifestyle of the microorganism community, $H_2$ availability, and the prevailing fluid-flow conditions in a reservoir determine whether that community is able to locate and prosper at the fluid-fluid interfaces within UHS (Zheng et al., 2021). Planktonic microorganisms are more likely to find fluid-fluid contacts/interfaces and flourish at those locations. They are helped in doing so by the hydrophilic tendencies of the extracellular polymeric substances (EPS) they secrete, forming their motile appendages. Their exploitation of EPS also enhances their ability to find and adhere to such interfaces.

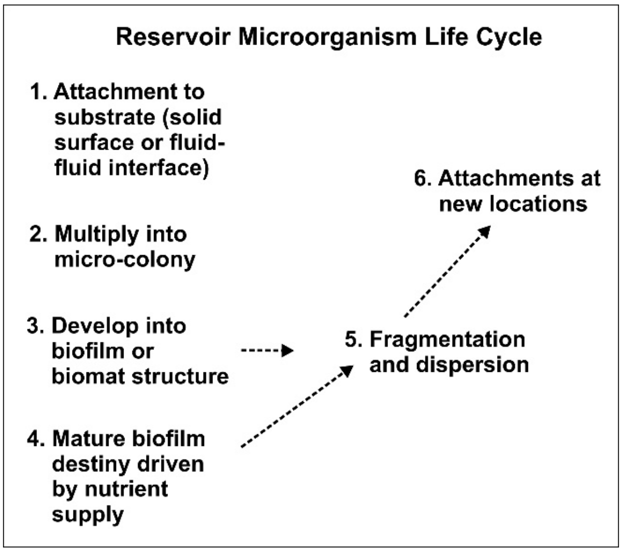

**Fig. 3.** Steps in the development and evolution of microorganism accumulations in porous reservoirs.

Cell shape and size (typically about one micrometer) cause many microorganisms to behave as colloids in fluid systems. The colloidal properties they display, such as motility and adhesion, vary according to their cell dimensions. At fluid-solid interfaces, hydrodynamic conditions (Liu et al., 2025), particularly fluid-flow rates (Krsmanovic et al., 2021), and surface roughness influence prevailing Eh, IFT, and CA conditions that impact microorganisms’ adhesion/detachment capabilities (Fig. 4). Those capabilities are determined by a complex interaction of multiple forces (Ali et al., 2023).

In summary, fluid-fluid and fluid-solid interfacial properties (e.g., interfacial tension, wettability, capillarity) strongly influence microorganism positioning, growth, and $CH_4$ generation in porous reservoir formations. They achieve this by controlling the positions of microorganism growth within the reservoir by determining the preferred

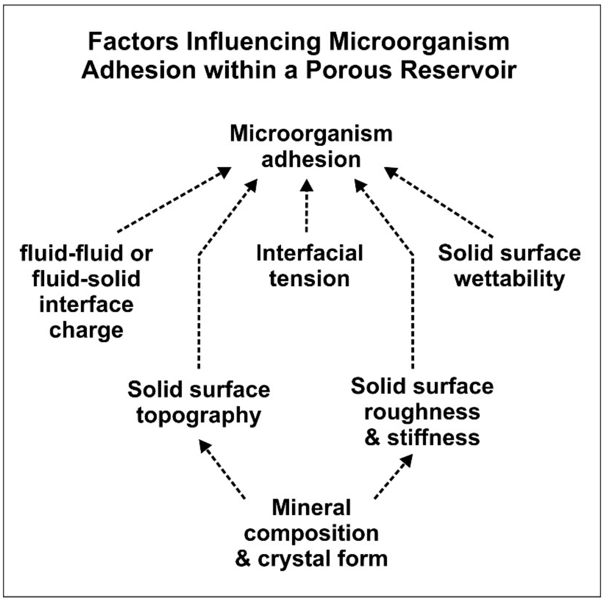

**Fig. 4.** Microorganism adhesion to interfaces is influenced by complex interactions of multiple factors.

sites for cell attachment and agglomeration. This, in turn, determines the locations in a reservoir where $CH_4$ generation is likely to be concentrated. Specifically, capillary forces determined by IFT and CA determine where microorganism cells choose to reside and develop within a reservoir (Black et al., 2025). Hence, interfacial properties play a key role in microorganism development within porous reservoirs, and, within limits, many microorganisms are able to adjust interfacial properties at fluid-fluid and fluid-solid interfaces to suit their metabolism.

At high fluid-flow rates, biofilms tend to become more heterogeneous due to local impacts of shear forces and variations in nutrient flow within their structures (Wheeler et al., 2019). When fluid-flow (shear-stress) reservoir conditions are low to moderate, biofilms tend to enhance their defences against detachment. They tend to do this by depositing more EPS, but this does not occur in turbulent conditions (Pizzi et al., 2025). Some microorganism displacement occurs independently of fluid-flow rate and is part of the dispersion mechanisms built into their life cycles. Biofilms may be prompted to release/detach cells in response to certain environmental changes or extreme conditions (e.g., a substantial reduction in nutrient supply).

## 3. Biomethanation in $H_2$ and $CO_2$ reservoirs

In UHS reservoirs, methanogenesis is an undesirable process, and steps are required to inhibit it. On the other hand, it can be a beneficial process in $CO_2$-storage reservoirs as it inhibits $CO_2$ migration to an extent. Hence, in some cases, it may be justifiable to inject $H_2$ and hydrogenotrophic methanogens into a $CO_2$-storage reservoir to promote it. Fig. 5 schematically illustrates the biomethanation process induced in a UCS reservoir. Up to 2025, only three countries (Argentina, Austria, and the Czech Republic) have conducted underground biomethanation field-scale tests (Wu et al., 2024).

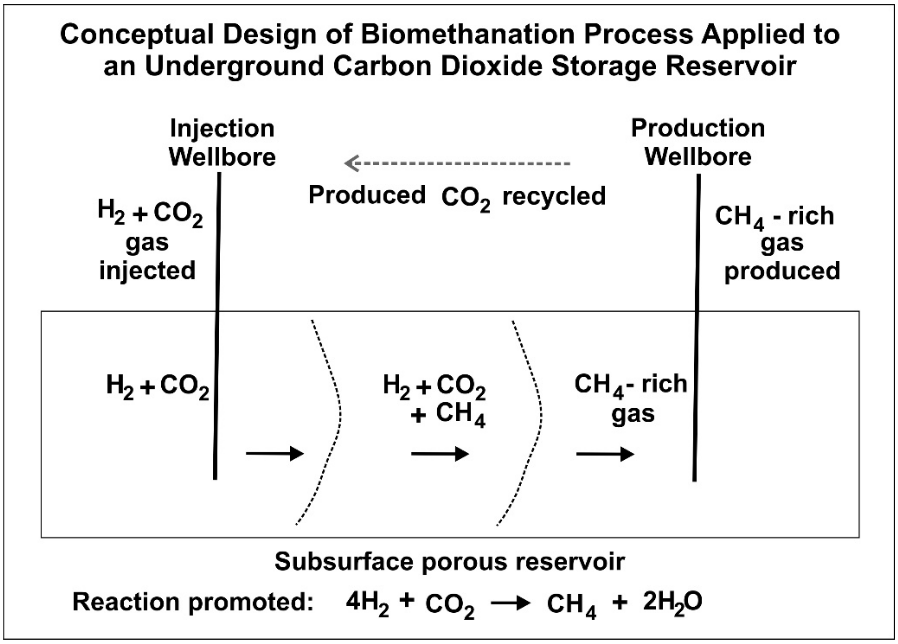

**Fig. 5.** Gas movements involved in the biomethanation of a UCS reservoir.

### *3.1 Methanogenesis in UHS reservoirs*

Based on laboratory-scale studies, Thaysen et al. (2021) estimated hydrogen transformation rates of up to 1205 nano molality/ hour (nm/h) at UHS-reservoir scales. This equates to a relatively low $CH_4$ formation reaction rate of 301 nm/h. However, Tyne et al. (2021) identified substantially faster methanogenesis over a 29-year period at the Olla $CO_2$-EOR field (Louisiana, USA). They determined using isotopic and gene-sequencing analysis that between 13% and 19% of the injected $CO_2$ retained in that reservoir had been transformed to $CH_4$ by methanogenesis. That natural transformation equates to between 73 and 109 millimoles of $CH_4/m^3/y$ (at standard T and P).

Wang et al. (2024) used single-cell simulations, configured with a $CO_2 : H_2$ molar ratio of 1.86 : 1 to enable up to 13% conversion of $H_2$ to $CH_4$ to match the observed Olla field methanogenesis outcome recorded over a 29-

year period. They found that a reaction rate of 1746 nm/h (frequency factor $1\times10^{-7}$) could convert 13% of the $H_2$ present in their simulation cell to $CH_4$ over a 29-year period, whereas faster reaction rates completed that conversion much more rapidly. A 1746 nm/h reaction rate is about twice the rate actually observed at the Olla field. On the other hand, slower reaction rates similar to those estimated by Thaysen et al. (2021), e.g., 296 nm/h (frequency factor $1.4\times10^{-7}$), generated much less $CH_4$ over the 29-year period. The simulation results also suggest that in UHS reservoirs with $CO_2$ cushion gas $H_2 : CO_2$ mixing and methanogenesis would be less in gravity-stable systems than in systems where flow conditions enabled more $H_2$ to enter the cushion gas by viscous fingering. Clearly, at relatively high methanogenesis rates, substantial amounts of stored $H_2$ in UHS reservoirs could be lost over the medium term. Moreover, the generation of water in the methanogenesis process could accelerate water breakthrough. Hence, methanogenesis poses a risk in UHS reservoirs depending on the rate at which the process occurs.

### *3.2 Exploiting biomethanation in $CO_2$ storage reservoirs*

Biomethanation in subsurface reservoirs involves promoting the processes by which microorganisms convert $H_2$ and $CO_2$ present in the reservoir fluids to $CH_4$. To successfully promote biomethanation in a subsurface reservoir, research suggests that moderate porosity (>10%) and permeability (>10 mD) are required, with reservoir conditions involving > 10% water saturation and 30 °C to 70 °C (Strobel et al., 2020). This rules out deeper reservoirs where temperatures exceed that upper temperature limit. There are several factors that potentially influence the performance of biomethanation (Fig. 6).

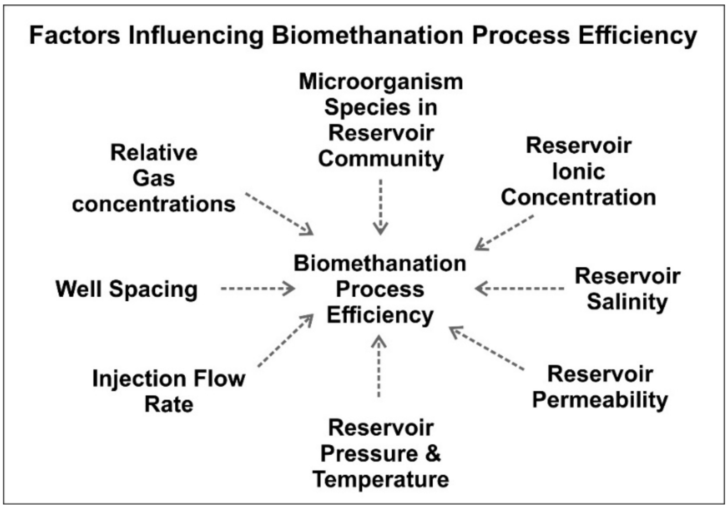

**Fig. 6.** Factors that potentially influence the biomethanation of a UCS reservoir.

Several potential benefits and risks are associated with initiating biomethanation in UCS reservoirs (Wu et al., 2023). The key potential benefits are: (1) enhancement of the rate at which carbonate minerals are formed, thereby increasing long-term $CO_2$-storage security; (2) restricting $CO_2$ mobility in the reservoir; thereby lowering the risk of leakage; (3) higher reservoir pH reducing the risk of corrosion; and (4) the generation of commercially exploitable quantities of $CH_4$ as a viable energy source in the long term. The key potential risks are: (1) increasing the development of sulfate-reducing (SRM) methanogens, thereby increasing corrosion; (2) increasing the formation of biofilms and pore clogging, thereby reducing reservoir permeability, wellbore injectivity rates, and reservoir storage capacity; and (3)Heterogeneous changes in reservoir fluid compositions throughout the reservoir making reservoir performance more difficult to monitor, simulate and predict over time.

Bioreactive transport models (BRT) assess microorganism growth/decay rates based on prevailing reservoir conditions experiencing multi-phase flow/displacement. To be effective BRT needs to consider the impacts of numerous processes impacting fluid flow within a reservoir, including non-isothermal flow, multiple biochemical reactions, molecular diffusion, and mechanically induced fluid dispersion. Often, simplistic assumptions are applied in BRT models regarding the various aspects of microorganism kinetics (i.e., growth rate, metabolism, survival rate, and environmental interactions) under a range of reservoir conditions. The Monod equation is often used to determine microorganism growth based on nutrient availability/concentration. Its formula results in growth rates progressing non-linearly with increasing nutrient concentration. The growth rate flattens out when nutrient concentration is sufficient to support the maximum growth rate of a specific microorganism species. Monod models are typically constrained by boundary conditions. In particular for UHS/UCS reservoirs, Dirichlet (fixed) boundary conditions are often applied for reservoir pressure, water saturation, temperature, salinity, or maximum gas concentrations. On the other hand, Neumann (derivative) conditions are also applied to capture time-variant molar fluxes flowing laterally through a reservoir in two or three dimensions.

Minougou et al. (2024) applied the Kozeny-Carman relation, which assumes porous medium approximate bundles of tortuous capillaries, to estimate permeability-porosity-specific surface area (SSA) relationships in terms of microorganism growth rates implied from $H_2S$ fluid concentrations. Their results indicated that as microorganisms consumed sulfide minerals in the substrate, porosity-permeability conditions in the near-wellbore regions were likely to become impaired. They simulated a UCS reservoir designed for biomethanation by varying the facility design and operating variables but assuming a simplistic microorganism assemblage and kinetics. The gas composition they evaluated (40% $H_2$; 10% $CO_2$; 50% $N_2$) was injected at 15 moles/s. Gas conversion rate into $CH_4$ and the cumulative quantity of $CH_4$ produced were tracked over a 30-year simulated period for injector and producer wells separated by 350 m. This enabled the $H_2$ conversion rate to be calculated.

Near-wellbore microorganism activity/growth can influence reservoir fluid flow conditions by altering porosity and permeability. If pore clogging materializes to a substantial degree, it can reduce wellbore gas injectivity loss, which would require costly remediation or well workovers. Hence, Minougou et al. (2024) configured their model to record variations in injectivity with distance from the injection well. Parametric sensitivity analysis was conducted by varying $H_2$ and $CO_2$ mole fractions, gas injection rate, reservoir pressure (P), and temperature (T). From year 0 to year 5, the simulation results revealed that biomass density increased in the vicinity of the injection well, accompanied by a reduction in permeability. Well spacing and $CO_2$ mole fraction were the most influential factors, followed by injection rate, with pressure and temperature exerting only limited influence. Their model identified that the lowest conversion rate to $CH_4$ occurred at specific $CO_2$ : $H_2$ mole fractions (5% : 45% and 20% : 30%), whereas the highest conversion rates occurred at other specific mole fractions (10% : 40% and 15% : 35%). Clearly, it would be necessary to optimize $CO_2$ : $H_2$ mole fractions in the gas mixture injected to maximize $CH_4$ production from biomethanation processes applied to specific reservoirs and reservoir conditions.

The many simplistic assumptions (e.g., microorganism kinetics and assemblage, constant reservoir porosity and permeability, Kozeny-Carman fluid dynamics property relationship assumptions) made in the Minougou et al. (2024) model, and other such simulations, limit their potential for extrapolation to real reservoir conditions. Future work is needed to consider the dynamics of a more complex microorganism assemblage and its influence on multi-phase fluid behavior under a broader range of heterogeneous reservoir conditions.

## 4. Bioreactive transport models

Bioreactive transport models (BRT) consider the reaction kinetics, fluid-flow dynamics, and interfacial consequences of microorganism colonization of subsurface porous formations. BRT models are relevant to UGS, UHS, and UCS reservoirs, the performance of which depends on multiple factors (Fig. 7).

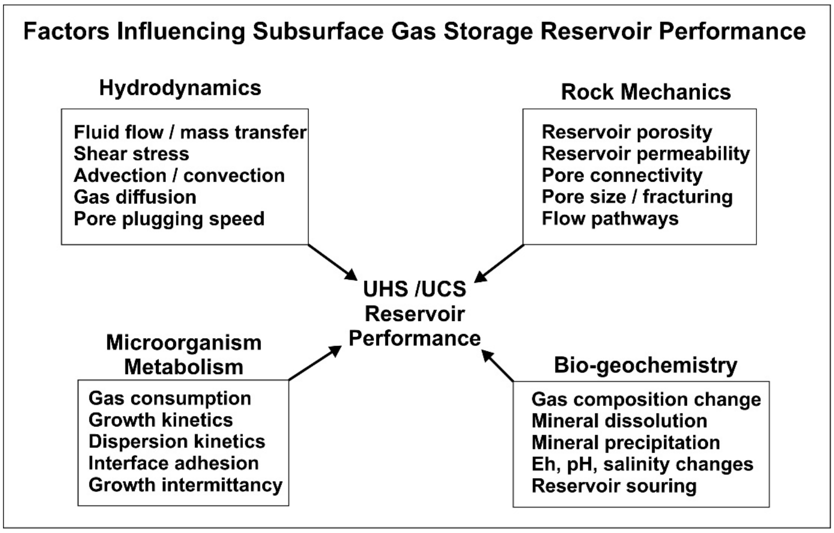

**Fig. 7.** Technical factors that influence UHS/UCS reservoirs and need to be considered by BRT simulations.

The abilities of microorganisms to move independently (motility), their capabilities to adhere to and grow on surfaces as individual species and/or microbial colonies (biofilms), and factors impacting microorganism metabolism (e.g., availability of essential nutrients) impact the long-term performance of UHS/UCS reservoirs. These microorganism characteristics may act to constrain or enhance methanogenesis and its mass transfer consequences, depending on the prevailing subsurface conditions. Much uncertainty remains concerning the abilities of complex microorganism communities in realistic subsurface conditions. For UHS systems, BRT models must consider the phase equilibria between $H_2$-rich gas and brine (formation water), considering gas mixtures that include $H_2$, $N_2$, $CH_4$, and $CO_2$ (if it is used as a cushion gas) (Ferrando et al., 2025). $H_2$ can be transported in reservoir conditions both in the vapor phase and dissolved in formation water, and its transport can be affected by advection, diffusion, and dispersion processes.

Historically, BRT models have tended to focus on modelling simple systems involving just a few well-studied microorganism species nurtured in laboratory conditions in model systems. The models tend to consider micro- (pore-scale) and macro- (reservoir scale) scales. However, the spatial and temporal dimensions of the reservoir considered tend to be limited, and only address heterogeneities superficially, if at all. While this approach simplifies the analysis and computational requirements, it makes most existing BRT models difficult to downscale or upscale. To improve those models such that they are relevant to long-term UHS/UCS systems, the models need to be configured in 3D to incorporate reservoir heterogeneities. Such 3D models are dimensionally large and computationally costly to evaluate.

Heterogeneity is difficult to incorporate into BRT simulations for two reasons. (1) For most subsurface reservoirs, limited data is available with which to characterize the detailed porosity and permeability variations throughout the reservoir. This is because most reservoirs are typically only penetrated and sampled by very few wells. Extrapolations are, therefore, necessary between wells, leading to substantial reservoir quality uncertainties. In reservoirs in which a large number of wells have been drilled, the reservoir quality uncertainty is less than that for reservoirs in which just a few wells have been drilled. (2) High computational cost is the other factor making it difficult and time-consuming to incorporate reservoir uncertainty into BRT reservoir simulations. Such models need to address variations in microorganism distributions and their metabolic kinetics throughout a heterogeneous reservoir. To do this effectively requires three-dimensional (3D) models that consider porosity and permeability variations on a fine grid involving many thousands of nodes distributed throughout the reservoir. Many input variables are required for such a 3D simulation to calculate the microorganism metabolism at each of these nodes. Consequently, most existing studies have elected to ignore reservoir and biofilm heterogeneities and instead developed only simplistic 1D or 2D BRT simulations.

To be of value BRT, models have to address microorganism interactions with the well-established multi-scale/multi-physics issues associated with sub-surface porous formations (Cai et al., 2022). Time scales varying from seconds to decades are relevant to UHS/UCS reservoir systems (Kapellos et al., 2015). The spatial scales considered also influence surface area impacts (Khajooie et al., 2024). The timeframes in which nutrients and other molecular-level materials move into and through biofilms from the surrounding media (often referred to as “substrate diffusion”) substantially influence biofilm development. Hence, BRT models need to be configured such that they can address a wide range of spatial and temporal scales. Despite the challenges, by integrating microorganism metabolic, interfacial development, and transport processes, BRT has the potential to identify the ways in which biofilms can influence the diffusion and mixing of various gases in UHS/UCS systems.

BRT models can be configured to consider UHS/UCS systems from two contrasting perspectives: how UHS/UCS operating conditions impact microorganism development and their impacts on the reservoirs, or how microorganism development impacts UHS/UCS efficiency and long-term operational viability. To be effective, the BRT models need to address the multiple processes that influence microorganism interactions with UHS reservoirs (Fig. 7). These include microorganism growth, dispersion and metabolism, the kinetics of those processes, fluid-fluid and fluid-solid interface property changes (e.g., IFT and CA), fluid flow, pore clogging (permeability impairment), reservoir souring and $H_2$ mass distribution changes. Fig. 8 identifies the typical inputs and outputs associated with meaningful BRT simulation models.

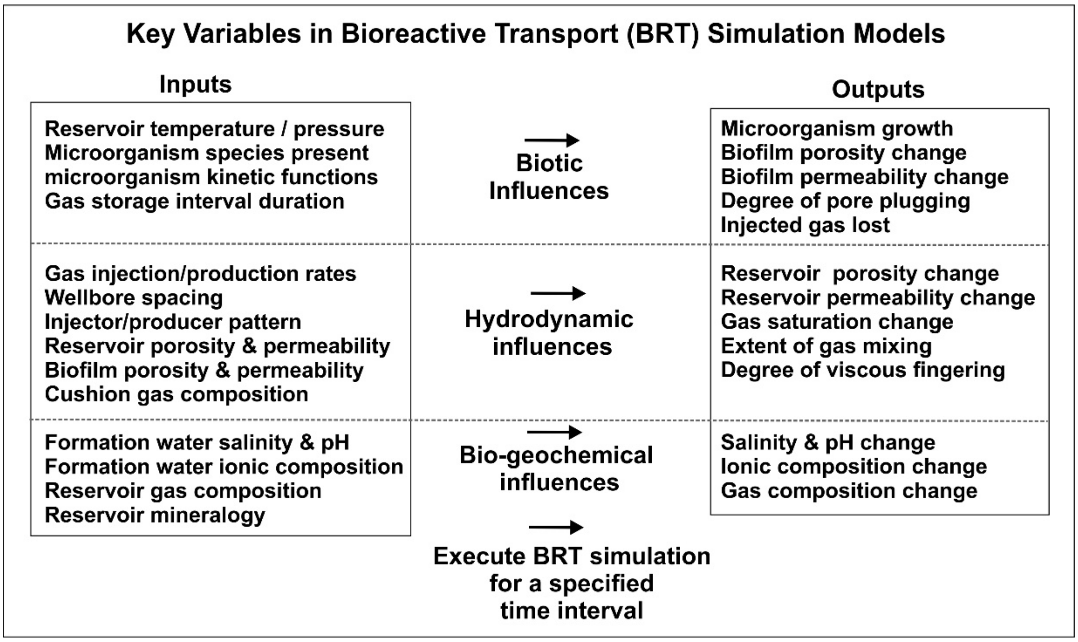

**Fig. 8.** Typical inputs and outputs required for meaningful bioreactive transport models.

The nature of fluid-flow in UHS/UCS systems (rate, fluctuations in rate and flow direction, and degree of intermittency) can have substantial impacts on microorganism development and their sustainability as biofilms at reservoir interfaces. Such conditions and long-term environmental influences are difficult to model and verify using only laboratory-scale testing equipment or simplified-system computer simulations, or surrogate models of those simulations complemented with machine-learning techniques. Hence, field-scale testing in pilot or fully-operational reservoirs has become a necessary part of the verification of BRT models. However, there are relatively few comprehensive simulations coupled with field tests of microorganism impact on UHS/UCS (Wu et al., 2024).

Hogeweg et al. (2024) developed a BRT kinetic reaction model for a simplified UHS system based on laboratory-scale reactor tests and the open-source DuMu$^x$ (DUNE for Multi-Physics framework, allowing for multiphysics simulations) simulator. Their model combined a fluid-flow (Darcy's Law) model, a double Monod Kinetic model, gas and liquid phase composed of nine components ($H_2O$, $CH_4$, $H_2$, $CO_2$, $C_2H_6$, $C_{3+}$ (pseudo-component), $N_2$, $SO_4^{2-}$, and $H_2S$), geochemical reaction models considering methanation, sulfate reduction (pyrite converted to pyrrhotite and generating $H_2S$), and gas solubility based on Henry's Law. Their simulations were for simplified, hypothetical UHS operations, configured to consider a series of $H_2$ injection and production cycles, and to predict $H_2$ loss and stored-gas purity changes over time. $H_2$ loss was broken down into permanent losses due to the reactions considered and temporary losses due to mixing between stored gas and cushion gas. Over a 1500-day simulated operating period, the model calculated that ~9.9% of the stored $H_2$ was permanently lost, taking into account all the combined reactions considered. The simplifying assumptions applied in that simulation model include a homogeneous reservoir, Darcy-equation flow, double Monod Kinetics, and a rock formation involving just three minerals (pyrite ($FeS_2$), pyrrhotite (FeS), and pure quartz ($SiO_2$). Hogweg et al. (2024) acknowledge that "real field tests are necessary to further develop and validate the model in a realistic subsurface environment".

Key simplifying assumptions made in the majority of existing BRT models are: (1) the reservoir modelled is continuous, homogeneous (constant porosity and permeability), and isotropic; (2) fluid-flow and nutrient delivery rates to biofilms are constant; (3) microorganism growth rates are governed by simple kinetic models (e.g., the classic Monod equation assuming that growth is dependent on a single substrate, or the double Monod model that takes two substrates into account). In real reservoirs, the formation tends not to be homogeneous, fluid- and nutrient-flow rates tend to fluctuate over time, and microorganism communities tend to consume multiple substrates simultaneously.

## 5. The critical role of reservoir interfaces in biofilm development

Microorganisms are typically unable to metabolize $H_2$ that does not reside as a dissolved phase in an aqueous fluid (Muñoz-Duarte et al., 2024). Hence, metabolic advantages exist in terms of access to consumable $H_2$ for biofilms to locate themselves at gas-liquid interfaces in UHS facilities where substantial mass transfer of $H_2$ occurs between gaseous and liquid phases. However, such interfaces tend to be discontinuous within porous media, so the microorganisms continually need to optimize their positions in relation to those interfaces.

The processes by which $H_2$ moves in bulk through a UHS reservoir vary depending on pore size and permeability (Lysyy et al., 2022). In tight reservoirs (low capillary numbers), $H_2$ tends to move dominantly by diffusion and is more likely to become trapped due to capillary forces. In such conditions, limited dissolution of $H_2$ occurs. In highly permeable formations (high capillary numbers), $H_2$ tends to move more extensively by advective and convective forces, with more bubble formation and $H_2$ mass transfer.

Two-dimensional BRT models indicate that microorganism growth becomes progressively slower as distance increases from the $H_2$-liquid interface due to diminishing nutrient supply (Strobel et al., 2023a). Indeed, certain microorganisms are guided chemically (chemotaxis) towards the negatively charged and low-viscosity gas-liquid contact and are able to effectively adhere to that interface. Hydrodynamic forces at the gas-liquid interface due to capillary pressure changes related to IFT gradients act to enhance adhesion (Ahmadzadegan et al., 2019). Enhanced microorganism activity concentrated at the gas-liquid contact typically leads to changes in IFT and increases in the interfacial area, which enhances $H_2$ mass transfer at those interfaces within biofilms (Krsmanovic et al., 2021).

Not all microorganisms are stabilized in biofilms and/or anchored to interfaces. High flow rates tend to increase detachment. Experiments have shown that certain sulfate-reducing bacteria are encouraged to detach and disperse from biofilms at high-$H_2$ conditions (Liu et al., 2025). In experimental conditions, multiple $H_2$ injections tended to increase the degree of biofilm detachment. Hence, biofilm behaviour seems to be species dependent and influenced by hydrodynamic conditions. Biofilms are more likely to expand during static reservoir conditions ($H_2$ not being injected or produced), increasing the risk of pore clogging of the reservoir, and/or corrosion risks to well-bore tubulars and increased $H_2S$ concentrations in the stored $H_2$.

At fluid-solid interfaces, wettability (contact angle, CA) influences capillarity and the ability of fluids to enter micropores. Certain microorganisms can alter CA, in either direction from initial conditions, through their EPS appendages. Some species do this by creating zones of modified hydrophobicity; others increase acidity that acts to dissolve certain minerals at the rock surface and change some of its physical properties (Park et al., 2020; Liu et al., 2023b). Microorganisms' ability to change CA at fluid-solid interfaces seems to be enhanced on smoother surfaces (Boon et al., 2024). It may also be impacted by changes in fluid salinity/pH. Experiments have observed that, as well as modifying substrate CA, microorganism activity at the fluid-solid interfaces can act to fragment $H_2$ gas clusters forming isolated gas bubbles (Liu et al., 2023b). This outcome is significant as it has the potential to disrupting existing $H_2$-flow channels and connectivity to wellbores.

## 6. Microorganism-induced reservoir consequences of concern

### *6.1 Reservoir souring by microorganisms*

Sulfate-reducing microorganisms (SRM) exploit a range of sulfur-containing compounds to generate $H_2S$, which simulations indicate can accumulate and modify IFT at UHS $H_2$-water interfaces and disrupt $H_2$-bubble stability (Chang et al., 2024). However, the presence of other gases coexisting at those interfaces may also influence the degree of IFT modification. Well-bore tubular corrosion is a key UGS/UHS/UCS risk of the $H_2S$ accumulated in the reservoir due to SRM activity (Wood, 2024a; Wood and Rezaee, 2025).

Anaerobic SRM tend to be involved in electrochemical reactions contributing to $H_2S$ production during the degradation of the metal surfaces (Pal et al., 2022). However, the process is complex and influenced by a range of environmental factors, and current knowledge of the community of SRM species involved in corrosion processes remains poorly understood (Xu et al., 2023), particularly in UHS reservoirs.

### *6.2 Microorganism-induced pore clogging*

In long-term $CO_2$-storage reservoirs, pore plugging by biofilms can have beneficial consequences by inhibiting $CO_2$ movements and potential leakage. Biofilm pore plugging can also be exploited in microbial improved and enhanced oil recovery from subsurface oil reservoirs to block unfavorable fluid migration routes (Wood, 2019). However, in operational UGS/UHS and UCS reservoirs, excessive pore clogging can substantially reduce reservoir porosity and permeability, which would ultimately degrade wellbore injectivity and productivity.

Eddaoui et al. (2021) developed a conceptual two-phase-flow numerical model to assess the impacts of pore clogging in UHS reservoirs due to the growth of biomethanation microorganisms, applying some simplifying assumptions. Their two-phase fluid-flow model involved a series of growth stages beginning with pore-wall attachments, followed by detachments resulting in partial or complete pore plugging with biomass. The results of their model indicated that progressive pore plugging inhibited vertical $H_2$ displacement in their conceptual UHS reservoir to an extent, whereas it promoted more extensive lateral/radial $H_2$ dispersal throughout the reservoir. However, the speed at which pore clogging occurs remains uncertain, as it would likely be influenced by variable nutrient concentrations in the pore space, progressively rising $H_2S$ concentrations, and several UHS operation conditions.

Microfluidic experiments with time-lapse imagery using model microorganism assemblages can be applied to monitor their growth through pore networks at micropore scales. Results of such experiments (Hassannayebi et al., 2021) have revealed a progression from initial colonization leading to subsequent growth, leading to variable flow/filtration-pathway development as the fluid-flow rates through the system are increased. The images generated were evaluated using Navier–Stokes–Brinkmann-flow simulations, which identified the intra-biomass permeability to be substantially higher than expected (> 300 mD). Their experimental and simulation outcomes for a range of in-biomass fluid-flow velocities indicated that advection would be the dominant intra-biomass flow mechanism controlling nutrient transport at permeabilities ≥ 10 mD. Those results imply that pore clogging does not necessarily destroy interstitial permeability but preserves intra-biomass permeability channels, allowing the passage of nutrients via advection, in addition to diffusion through growing biofilms. Such conditions would be expected to sustain ongoing biomass growth.

### *6.3 Mineral precipitation or dissolution generated by microorganisms*

Certain microorganisms can employ processes that result in mineral precipitation. For instance, $H_2$-oxidizer microorganisms can use traces of oxygen (where present as an injected gas impurity) or nitrates as electron receptors in $CO_2$ and $CH_4$ underground storage reservoirs (Vu et al., 2018; Haddad et al., 2022). The actions of such microorganisms can lead to deposition of oxides and sulfates on a reservoir formation's mineral grains. Other microorganisms can enhance carbon mineralization in carbon storage reservoirs (Starnoni and Sanchez-Villa, 2014).

On the other hand, the metabolisms of other microorganism species can result in mineral dissolution from the pore walls (Wu et al., 2024). The mineralogy and formation-water compositions at specific UHS sites influence the biochemical and geochemical reactions associated with mineral precipitation/dissolution. Shojaee et al. (2024) experimentally evaluated UHS systems involving a $CH_4$ cushion gas, a North Sea seawater composition as formation water, and calcite, dolomite, and quartz as individual mineral phases or as a collective mineral assemblage. They found that hydrogen loss was substantially greater in the dolomite systems and that changes in pH were the driver for that. Consumption of bicarbonate and hydrogen ions by the biochemical reactions upset the equilibrium of geochemical reactions in the systems evaluated. However, it is very difficult to model such complex reactions in 2D or 3D reservoir models.

## 7. Pore-scale reactive transport modelling of microorganism activities in UHS

### *7.1 Model concepts and assumptions*

BRT models for UGS/UHS/UCS reservoirs typically combine sets of equations with simplifying assumptions representing several physical processes. Each process addresses one aspect of microorganisms' influences on a reservoir fluid dynamics and stored gas compositions and quantities over time, considered at various scales (Li et al., 2025). The processes typically modelled include reservoir fluid flow, microbial growth (distinguishing between planktonic and biofilm accumulations), diffusion and advection of materials into and out of pore wall minerals, nutrient supply, and biofilm displacement kinetics. Many models are conducted at the pore scale, considering the biofilm as a continuous porous medium (Dawi et al., 2024).

Considering a biofilm as a micro-continuum circumvents, to an extent, the need to define its complex boundaries/interfaces. Such models typically apply the Monod growth rate kinetics equations to calculate biofilm growth and nutrient supply (Wu et al., 2024). In cases where mixtures of two stored gases are considered, a double Monod model is typically applied, e.g., for $H_2$ and $CO_2$ as the available substrates in a UHS system (Strobel et al., 2023b). However, there are at least seven different kinetic growth models that have been developed for application to microorganism metabolism (Vasile, 2024). The alternative equations expand upon the basic Monod equation but tend not to be configured to consider the involvement of multiple substrates. For example, the Moser kinetic growth model (Tan et al., 1994) adds an exponent to the substrate concentration, making the growth rates applied more flexibly controlled. On the other hand, the Panfilov kinetic model (Wu et al., 2024) addresses population dynamics in relation to fluid/nutrient flow and applies a maximum population size to microorganism growth.

It is sometimes useful to monitor the irregularity and intermittency of pore clogging in biofilms and how that influences nutrient flow pathways and flow rates. Kurz et al. (2022) found, based on microfluidic experiments, that microorganism growth typically competes with shear stresses in porous media, leading to substantial intermittency in fluid flow and nutrient supply as the degree of pore clogging varies. While such models provide useful information, they tend not to consider reservoir or biofilm heterogeneities. BRT models configured in this way are typically evaluated for a range of environmental conditions (fluid-flow rate, nutrient supply, pressure, salinity, temperature). The BRT models, configured as described, are frequently executed as simulations focused on specific scales (typically microscale and macroscale) or, in a few cases, multiple scales using various established software packages (Vasile, 2024).

### *7.2 Dual-porosity models*

Dual-porosity models (two separate equations) have been usefully applied considering two distinctive reservoir zones (e.g., the mobile fluid phase, and an immobile biofilm phase). These establish distinct mass-balance equations for each zone. A third equation then defines the mass transport (diffusion or advection) between the two zones to translate the pore-scale models into a macroscale system model. Such models outperform those attempting to represent such a system as a single equation. Orgogozo et al. (2013) developed such a model, considering 2D pore geometry of a biofilm zone to evaluate equilibrium and non-equilibrium conditions at the macroscale. Hagemann et al. (2024) developed a simplified analytical solution of a dual-porosity BRT model for UHS/UCS biomethanization system to evaluate the spatial distribution of $H_2$ and $CH_4$ throughout the reservoir in 3D over time. By considering two distinct systems: (1) involving advection plus dispersion, and (2) involving just advection, they found that the analytical solution with dispersion was able to closely replicate the more complex numerical solution. Such models have the potential, when developed with less simplistic assumptions, to be of value for optimizing well positioning and spacing in UHS/UCS reservoirs. Experimental evidence suggests that injection cycling in UHS reservoirs is able to create a near-wellbore dry-out zone that inhibits biomass growth, thereby reducing pore clogging and improving permeability and injectivity in the near-wellbore reservoir zones (Eddaoui et al., 2021; Bijay et al., 2024).

Cyclic injection of $H_2$ into UHS reservoirs creates dry-out zones surrounding injection wells. These are created by a combination of evaporation and capillary-displacement mechanisms that inhibit biofilm formation and mineral-salt deposition (Ghaedi et al., 2025). The injection of dry $H_2$ causes much of the formation water in the near-well-bore reservoir zone to evaporate. This forms an $H_2O$-gas phase and increases the salinity of the fluids remaining in the pore space. The water vapor is either flushed from that space further into the reservoir or produced with the $H_2$ during the production cycle. This drying process is perpetuated during each injection cycle. In addition, injected $H_2$ is the non-wetting phase in a water-wet reservoir formation, displacing water from the larger pore spaces as it is injected. Although some highly saline residual water is initially retained in the smaller pore spaces by capillary forces, repeated injection cycles gradually overcome those forces holding that water in place. Ultimately, the near-well-bore regions become a relatively dry zone dominated by $H_2$ with very small quantities of liquid formation water. In such a high-saline, dry-zone environment, microorganism growth, mineral salt deposition, and related pore clogging are inhibited in the large pore spaces and flow channels. By carefully scheduling the repeated $H_2$-injection cycles, UHS operators can perpetuate and control the near-well-bore dry zone to inhibit biofilm growth and mineral-salt deposition. This maintains those critical zones of a UHS reservoir free from pore clogging, with biofilm formation displaced further into the reservoir.

### *7.3 Verification of model results*

A key problem with simplified BRT models based on laboratory conditions is that they do not reflect the environmental conditions and heterogeneities likely to be encountered in actual UHS reservoirs. Moreover, they tend to consider a much narrower range of microorganism species and communities than are known to exist in subsurface environments. In a case where such models have been evaluated in conjunction with observations in an operating UGS systems (e.g., Lobodice UGS in Czech Republic), they were found (Tremosa et al., 2023) to work only when the biomethanization reactions were carefully calibrated to the reaction kinetics applicable to that specific reservoir. This suggests that simple dual-porosity BRT are not generalizable across multiple UGS/UHS/UCS reservoirs but need to be kinetically calibrated to the microbial communities present at individual reservoir sites.

Microorganism community activity tends to vary substantially over time, with intermittent swings in activity depending upon environmental conditions. Models that assume continuous biomass growth exhibiting strong positive correlations with $H_2$ consumption over time can be oversimplistic. Where environmental conditions change, in particular $P$, $Sa$, $T$, and fluid-flow rate/hydrodynamics with UHS/UCS operating conditions, biomass growth and $H_2$ consumption may fluctuate considerably.

## 8. Machine learning coupled with BRT models

Several studies have used machine learning (ML) to predict various physical properties of UCS and UHS reservoirs. Ansari et al. (2022) used ML models to predict $H_2$ solubility in water in terms of pressure ($P$), temperature ($T$), and salinity ($Sa$), whereas Longe et al. (2024) predicted $H_2$ solubility in water in terms of $P$, $T$, $Sa$, and salt type using deep-learning models coupled with optimizers applied to a larger dataset. Vo Thanh (2026) combined physics-informed machine learning (PIML) associated with an XGBoost model to predict $H_2$ solubility in terms of $P$, $T$, and $Sa$ and physical relationships impacting gas-liquid systems (e.g., Henry's law, Setchenow effect related to salinity, and gas compressibility).

Zhu et al. (2022) predicted hydrogen dissolution in brine in terms of $P$, $T$, and NaCl molality using a wavelet neural network. Ng et al. (2022) predicted IFT of $H_2$-brine systems in terms of $P$, $T$, and NaCl molality with a neural network using a small dataset. Gbadamosi et al. (2024) predicted IFT of $H_2$-brine systems in terms of $P$, $T$, and density difference using a Gaussian process regression model. Ahmadi (2025) applied a physics-informed neural network (PINN) to predict IFT in gas ($H_2$, $CH_4$, $CO_2$)-brine systems in terms of $P$, $T$, $Sa$, and gas composition. Longe et al. (2026) applied a deep learning optimizer model to 2676 laboratory tests to predict IFT in gas ($H_2$, $CH_4$, $CO_2$)-brine systems in terms of $P$, $T$, $Sa$, and gas composition. Vo Thanh et al. (2023) developed an XGBoost model to predict substrate wettability based on $P$, $T$, $Sa$, and substrate type (a range of minerals and rocks: sandstone, basalt, shale, quartz, dolomite, anhydrite, calcites, granite, gypsum, coal, and mica) in an $H_2$-brine system based on 513 laboratory tests. Omeke et al. (2025) developed a Fourier-integrated hybrid neural framework to model the dynamics of UHS injection-withdrawal cycling and its influences on reservoir fluid movements, including the spatial and temporal prediction of sharp fronts and abrupt changes in reservoir flow conditions.

Notably, none of the UHS ML studies mentioned consider microorganism impacts on the reservoir properties considered. This makes them of limited to value for assessing those physical properties in real UHS reservoirs. As more data becomes available, it should be possible to apply ML models to predict certain BRT model parameters or serve as surrogate models for more complex and time-consuming simulations.

## 9. Potential for future research and development

Substantial potential remains to improve understanding and modelling of gas storage performance in UCS and UHS reservoirs. Four key areas worthy of more detailed attention are:

(1) Expanding the capabilities of BRT models to address more complex 3D systems. These should include heterogeneous reservoir conditions, intermittent biofilm development, more diverse communities of microorganisms, growth and dispersion kinetics tailored to varying environmental conditions and microorganism communities, and taking account of evolving mixed stored gas compositions.

(2) Expanding the use of ML, in particular physics-informed machine learning (Fig. 9), as surrogate models for BRT simulations to more efficiently estimate microorganism-induced physical-property changes for a wide range of UCS and UHS reservoir conditions. Recent developments in physics-informed machine learning (Davoodi et al., 2026) suggest that physics-guided machine learning is best suited for modelling subsurface reservoirs impacted by a high degree of heterogeneity.

(3) There is substantial potential to evaluate and apply the CRISPR gene editing technique and its variants to improve (in the case of UCS) or degrade (in the case of UHS) the efficiency of the $CH_4$ generation by hydrogenotrophic microorganisms. Such gene editing techniques have been successful in modifying aerobic methanotrophic bacteria (Rumah et al., 2023) and the archaeon Methanococcus maripaludis (Du et al., 2024). Gene editing technologies have been applied extensively over the past decade to improve the growth rates and lipid yields of microalgae (Wood, 2022), and there are likely to be benefits in applying these techniques to each group of microorganisms identified in Fig. 1.

(4) Expand the use of DNA sequencing to more comprehensively characterize the microorganism communities present in potential and actual UHS reservoirs (Belcour et al., 2025), and their expected $H_2$ consumption (Cerna et al., 2025). Once extensive databases are established covering multiple UHS reservoirs, it should be possible to promptly identify the most active microorganism types in those reservoirs and quantify the risks of gas loss, corrosion, and pore clogging more realistically.

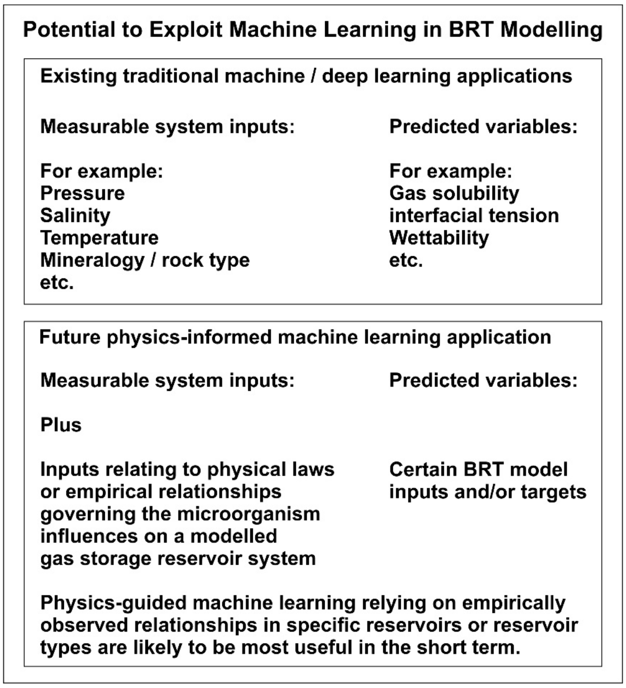

**Fig. 9.** The potential for physics-informed machine learning to assist bioreactive transport modellingin the future.

## 10. Conclusions

The microorganism impacts on underground hydrogen storage (UHS) and carbon dioxide storage reservoirs (UCS) are evaluated in terms of how they influence the evolution of stored gas compositions, reservoir porosity, permeability and mineralogy, and fluid dynamics. The risks of stored gas losses and wellbore-tubular corrosion are also considered. The actions of multiple types of microorganisms are distinctive and result in relatively predictable qualitative reservoir outcomes based on historical experimental studies and simplified-system simulations. However, quantifying these changes with models configured at the reservoir scale is difficult because there are so many complex variables and reservoir and biofilm development heterogeneities that impact the outcomes of interest. Most existing bioreactive transport

(BRT) models/simulations are based on laboratory studies applying substantially simplified assumptions regarding the key variables and the microorganism growth kinetics. The majority of those models are not validated with real UHS/UCS field tests nor do they consider realistic subsurface reservoir environments. Existing models typically ignore reservoir heterogeneities and fail to consider the diverse microorganism communities that exist in real subsurface reservoirs.

Substantial progress has been made in recent years in understanding the processes involved in biomethanation, identifying the potential to exploit that process in UCS reservoirs. This can be achieved by co-injecting $H_2$ and $CO_2$ into UCS reservoirs to generate recoverable methane and potentially improve the stability of stored $CO_2$ in UCS reservoirs. Progress has also been made in genetic sequencing (metabarcoding) for characterizing the microorganism communities in reservoir brines, making it possible to rapidly predict the dominant microorganism activities and the injected gas composition changes, most likely to occur in specific reservoirs. To date, machine learning (ML) has not been used to support BRT modelling, but there is substantial potential for future use, particularly in the form of physics-informed machine learning (PIML). ML and PIML techniques offer the potential to exploit the growing databases of genetically based characterization of the UHS and UCS microorganism communities. There is also potential to use CRISPR gene-editing techniques to improve the performance of specific microorganisms. This could be performed with the objective to mitigate some of the adverse consequences in UHS reservoirs (e.g., pore clogging and corrosion) or to further exploit some of the benefits (e.g., biomethanation) in UCS reservoirs.

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