International Journal of Environmental Sciences
ISSN: 2229-7359
Vol. 9 No. 1s, 2023
https://theaspd.com/index.php

Numerical Modelling of Reactive Transport in Geothermal Reservoirs for Long-Term Performance Prediction

Milicent Okyere Williams
Ghana National Gas Company Limited

Abstract
Numerical modelling of reactive transport has become a critical tool for understanding and predicting the long-term performance of geothermal reservoirs under sustained exploitation. By coupling fluid flow, heat transfer, and geochemical reactions, reactive transport models enable the assessment of how mineral dissolution, precipitation, and porosity–permeability evolution influence reservoir productivity over time. This study reviews and synthesizes established and emerging numerical approaches for simulating reactive transport processes in geothermal systems, with particular emphasis on their role in forecasting thermal decline, injectivity changes, and sustainability under production and reinjection scenarios. Advances in three-dimensional modelling, high-performance computing, and hybrid physics-based–data-driven frameworks are examined, highlighting their contribution to improving predictive capability while managing computational cost. Application examples from sedimentary, volcanic, and enhanced geothermal systems illustrate the practical relevance of reactive transport modelling for long-term resource management. Remaining challenges related to scale effects, parameter uncertainty, and model validation are discussed, outlining directions for future methodological development and operational integration.
Keywords: *Reactive transport modelling, Geothermal reservoirs, Long-term performance prediction, Thermo-hydro-chemical processes, Numerical simulation, Reservoir sustainability.*

1. INTRODUCTION

Geothermal energy represents a reliable and low-carbon renewable resource capable of providing baseload power and direct heat over extended operational lifetimes. However, the long-term performance of geothermal reservoirs is governed by complex interactions among fluid flow, heat transfer, and geochemical reactions occurring within porous and fractured subsurface formations. As geothermal systems are subjected to sustained production and reinjection, these coupled processes can induce significant changes in reservoir temperature distribution, mineralogical composition, porosity, and permeability, ultimately influencing productivity and sustainability (Blöcher et al., 2010; Mottaghy et al., 2011; Sonney & Vuataz, 2009).
Traditional thermal–hydraulic models, while effective in capturing pressure and temperature evolution, often neglect the role of geochemical reactions that may lead to scaling, clogging, or dissolution-induced permeability enhancement. Early coupled thermal–hydraulic–chemical (THC) studies demonstrated that mineral–fluid interactions can substantially alter reservoir properties over operational timescales, highlighting the necessity of incorporating reactive transport processes into geothermal reservoir simulations (Bächler & Kohl, 2005; Kühn et al., 2002). Reactive transport modelling (RTM) provides a physically consistent framework to simulate the simultaneous transport of heat and chemical species alongside kinetically and thermodynamically controlled reactions, offering deeper insight into reservoir evolution under exploitation conditions (Alt-Epping & Diamond, 2008; Xiao & Jones, 2018).
In recent years, RTM has been increasingly applied to a broad range of geothermal contexts, including sedimentary geothermal systems, volcanic reservoirs, and enhanced geothermal systems (EGS). Case studies from Europe, New Zealand, and elsewhere demonstrate the value of three-dimensional reactive transport simulations for forecasting temperature decline, evaluating reinjection strategies, and assessing long-term resource renewability (Kühn & Stöfen, 2005; Bujakowski et al., 2016; Torresan et al., 2022). Furthermore, RTM has proven essential for understanding chemically induced changes arising from stimulation treatments and CO_2-rich fluid circulation, where mineral dissolution and precipitation strongly affect reservoir performance and integrity (Aradóttir et al., 2012; Ma et al., 2023; Alt-Epping et al., 2013).
Despite their predictive power, fully coupled reactive transport models remain computationally demanding and subject to uncertainty arising from parameter estimation, scale transitions, and limited availability of long-term field data (Abd & Abushaikha, 2021; Egert, 2021). To address these challenges, advances in

numerical methods, high-performance computing, and hybrid modelling approaches have gained prominence. GPU-accelerated simulators and unstructured mesh frameworks enable field-scale, three-dimensional simulations with evolving porosity and permeability (Fowler et al., 2016; Sohrabi et al., 2019), while reduced-order models and machine-learning-based surrogates offer promising pathways for efficient long-term performance prediction (Mudunuru et al., 2017; Jiang et al., 2022, 2023; Demirer et al., 2023).
Against this backdrop, this article examines the role of numerical modelling of reactive transport in predicting the long-term performance of geothermal reservoirs. By synthesizing advances in coupled process modelling, computational techniques, and data-driven methods, the study highlights current capabilities, limitations, and future directions for improving the reliability of geothermal resource assessment and sustainable energy production.

2. Fundamentals of Reactive Transport in Geothermal Reservoirs

Reactive transport processes play a central role in controlling the long-term behavior and performance of geothermal reservoirs. These processes arise from the complex coupling between fluid flow, heat transfer, solute transport, and geochemical reactions occurring within porous and fractured subsurface formations. In geothermal systems, the circulation of high-temperature fluids induces mineral dissolution and precipitation, alters porosity and permeability, and modifies fluid composition, all of which directly influence reservoir productivity and sustainability over time (Alt-Epping & Diamond, 2008; Kühn et al., 2002). Numerical modelling of reactive transport therefore provides a physically consistent framework for understanding and predicting reservoir evolution under natural conditions and during prolonged energy exploitation (Blöcher et al., 2010; Mottaghy et al., 2011).

2.1 Governing Physical and Chemical Processes

Reactive transport in geothermal reservoirs is governed by the simultaneous interaction of thermal, hydraulic, chemical, and, in some cases, mechanical processes. Fluid flow is driven by pressure gradients and buoyancy forces induced by temperature-dependent density variations, while heat is transported through advection and conduction (Bundschuh & Arriaga, 2010). The transport of dissolved chemical species occurs through advection, diffusion, and dispersion, providing the basis for geochemical reactions between fluids and the surrounding rock matrix (Xiao & Jones, 2018).
At elevated geothermal temperatures, reaction kinetics are significantly accelerated, enhancing mineral dissolution and precipitation rates. These reactions can lead to changes in fluid chemistry, scaling within wells, or alteration of reservoir rock properties (Alt-Epping et al., 2013). The tight coupling between flow, heat, and chemistry distinguishes geothermal reactive transport systems from conventional groundwater systems and necessitates fully coupled numerical formulations (Bächler & Kohl, 2005; Kühn & Stöfen, 2005).

2.2 Mathematical Formulation of Reactive Transport Models

Reactive transport models are typically formulated as systems of coupled, nonlinear partial differential equations representing mass conservation of fluids, energy balance, and species transport, combined with algebraic or kinetic expressions for geochemical reactions (Abd & Abushaikha, 2021). The mass balance equations describe multiphase or single-phase fluid flow in porous or fractured media, while energy equations account for temperature evolution within the reservoir (Bartels et al., 2005).
Geochemical reactions may be represented using equilibrium, kinetic, or mixed approaches depending on the timescales of interest and data availability. Equilibrium reactions are often applied to fast-reacting mineral systems, whereas kinetic formulations are required to capture time-dependent dissolution and precipitation processes relevant for long-term geothermal forecasting (Alt-Epping & Diamond, 2008; Aradóttir et al., 2012). The resulting mathematical system is highly nonlinear and computationally demanding, particularly when porosity–permeability feedbacks are included (Sohrabi et al., 2019).

Table 1: Key Components and Processes in Reactive Transport Modelling of Geothermal Reservoirs

Model Component	Physical Meaning	Impact on Reservoir Performance
Fluid Flow	Movement of geothermal fluids through porous and fractured media	Controls circulation patterns, recharge efficiency, and pressure drawdown,

	driven by pressure gradients and buoyancy effects	directly influencing sustainable heat extraction rates
Heat Transport	Transfer of thermal energy via conduction and advection within the reservoir	Determines thermal breakthrough timing, reservoir cooling rates, and long-term energy production potential
Solute Transport	Migration of dissolved chemical species in geothermal fluids	Influences fluid chemistry evolution, scaling risk, and availability of reactants for mineral reactions
Mineral Reactions	Dissolution and precipitation processes between fluids and rock-forming minerals	Alters fluid composition and solid volume fractions, affecting permeability, injectivity, and long-term reservoir stability
Porosity–Permeability Evolution	Changes in pore space and flow capacity resulting from mineral reactions	Governs feedback mechanisms that can enhance or degrade reservoir performance through permeability enhancement or clogging

2.3 Numerical Discretization and Solution Strategies

Due to the complexity of reactive transport equations, numerical solutions rely on spatial and temporal discretization techniques such as finite difference, finite volume, and finite element methods (Fowler et al., 2016). Structured grids are commonly used for simplified reservoir geometries, whereas unstructured meshes enable more realistic representation of geological heterogeneity and fracture networks (Sonney & Vuataz, 2009).

Time integration schemes must balance numerical stability and computational efficiency, particularly for stiff geochemical systems. Operator splitting techniques are frequently employed to decouple transport and reaction steps, although fully coupled approaches provide improved accuracy for strongly interacting processes (Gherardi et al., 2012). Advances in parallel computing and GPU acceleration have significantly enhanced the feasibility of three-dimensional, field-scale reactive transport simulations (Sohrabi et al., 2019).

2.4 Porosity–Permeability Evolution and Feedback Mechanisms

One of the defining features of reactive transport in geothermal reservoirs is the dynamic evolution of porosity and permeability induced by mineral reactions. Dissolution processes can enhance permeability and improve fluid circulation, whereas precipitation may reduce pore space, leading to flow channeling or clogging near injection and production wells (Kühn et al., 2002; García-Gil et al., 2016).

Accurately capturing these feedback mechanisms is essential for long-term performance prediction, as small changes in permeability can result in substantial variations in heat extraction efficiency (Parisio et al., 2019). Numerical models increasingly incorporate empirical or physics-based relationships linking mineral volume changes to hydraulic properties, although uncertainty remains a major challenge (Egert, 2021).

2.5 Scale Effects and Model Parameterization

Reactive transport processes operate across a wide range of spatial and temporal scales, from pore-scale mineral reactions to reservoir-scale thermal depletion over decades (Alt-Epping & Diamond, 2008). Upscaling laboratory-derived kinetic parameters to field-scale models remains a key source of uncertainty, particularly in fractured geothermal systems (Abd & Abushaikha, 2021).

Parameterization of reactive transport models typically relies on a combination of core experiments, well logs, geochemical analyses, and inverse modelling techniques (Blöcher et al., 2010; Torresan et al., 2022). Sensitivity analyses are commonly employed to assess the influence of uncertain parameters on model predictions and to guide data acquisition strategies during reservoir operation (Erol et al., 2023).

In sum, the fundamentals of reactive transport in geothermal reservoirs are rooted in the tight coupling between fluid flow, heat transfer, and geochemical reactions, which collectively govern reservoir evolution and long-term performance. Numerical reactive transport models provide a robust framework for integrating these processes and evaluating sustainability under prolonged exploitation. Despite advances in mathematical formulation, numerical methods, and computational power, challenges remain in parameter uncertainty, scale transitions, and model validation. Continued refinement of reactive transport modelling approaches is therefore essential for reliable long-term prediction and sustainable management of geothermal resources.

3. Numerical Frameworks and Modelling Approaches

Numerical modelling has become an indispensable tool for understanding the complex interactions within geothermal reservoirs, particularly when assessing long-term performance. Reactive transport in geothermal systems involves the simultaneous simulation of heat transfer, fluid flow, and geochemical reactions, which collectively influence reservoir sustainability and productivity (Blöcher et al., 2010; Bächler & Kohl, 2005). Accurate numerical frameworks provide insight into spatial and temporal variations in temperature, pressure, and mineralogy, enabling operators to optimize production while minimizing environmental and operational risks (Mottaghy et al., 2011; Alt-Epping et al., 2013). This section discusses the main numerical modelling approaches, including governing equations, discretization methods, coupled processes, and recent computational advancements.

3.1 Governing Equations in Reactive Transport Modelling

Reactive transport modelling (RTM) relies on a set of coupled partial differential equations (PDEs) representing fluid flow, heat transfer, and geochemical reactions. Fluid flow is typically described using Darcy's law for porous media, while energy transport is modeled through the heat conduction–convection equation. Geochemical reactions, including dissolution, precipitation, and adsorption, are integrated using mass balance equations for reactive species (Xiao & Jones, 2018; Abd & Abushaikha, 2021). The general form of the coupled equations can be expressed as:

$$\frac{\partial(\phi C_i)}{\partial t} + \nabla \cdot (\mathbf{v} C_i - D \nabla C_i) = R_i$$

where ϕ is porosity, Ci is species concentration, v is fluid velocity, D is the diffusion-dispersion tensor, and Ri represents the net reaction rate (Aradóttir et al., 2012; Ma et al., 2023).

This approach ensures that changes in porosity and permeability due to mineral reactions are dynamically captured, providing a realistic prediction of reservoir evolution under prolonged production and reinjection (Torresan et al., 2022; Sohrabi et al., 2019).

3.2 Discretization and Numerical Solution Techniques

Discretization of the governing PDEs is crucial for numerical solution stability and accuracy. Finite difference, finite element, and finite volume methods are widely used to approximate spatial and temporal derivatives in geothermal RTM (Bundschuh & Arriaga, 2010; Fowler et al., 2016).

- **Finite Difference Methods (FDM):** Suitable for regular grids and simple geometries; widely used in early geothermal reservoir simulations (Blöcher et al., 2010).
- **Finite Element Methods (FEM):** Flexible for complex geometries and heterogeneous reservoirs; particularly useful in 3D simulations of fractured media (Alt-Epping & Diamond, 2008; Kühn & Stöfen, 2005).
- **Finite Volume Methods (FVM):** Conserves mass locally and handles highly nonlinear reactions effectively, making it suitable for large-scale field applications (Sohrabi et al., 2019).

Time-stepping schemes, such as implicit or semi-implicit methods, are employed to maintain numerical stability when simulating stiff reactive systems with rapid mineral precipitation or dissolution reactions (Demirer et al., 2023).

3.3 Coupled Multi-Physics Modelling

Geothermal reservoirs require the integration of multiple physical processes. Multi-physics models explicitly couple fluid flow, heat transfer, and reactive transport to capture feedback mechanisms such as porosity-permeability evolution due to mineral dissolution or scaling (Bächler & Kohl, 2005; Parisio et al., 2019).

- **Thermal–Hydraulic–Chemical (THC) Coupling:** This approach enables the simulation of both energy extraction and geochemical interactions, which are critical in enhanced geothermal systems (Mudunuru et al., 2017; Altar et al., 2023).

- **Fractured vs. Porous Media Modelling:** Fractured reservoirs require discrete fracture networks integrated into continuum models, whereas porous systems can often be approximated with homogenized properties (Kühn et al., 2002; Sonney & Vuataz, 2009).

Table 2: Comparative Overview of Multi-Physics Modelling Approaches in Geothermal RTM

Approach	Advantages	Limitations	Typical Applications
THC Coupled FEM	Handles complex geometries; robust for chemical feedback	High computational cost	EGS and sedimentary reservoirs
FVM Coupled	Mass-conserving; stable for stiff reactions	Grid-dependent accuracy	CO_2 injection and mineral scaling studies
Hybrid Data-Driven	Reduces simulation time; predictive analytics	Requires training datasets	Real-time thermal output forecasting

3.4 High-Performance Computing and Scalability

Field-scale RTM often requires solving millions of coupled equations, necessitating high-performance computing (HPC) frameworks. GPU-based parallelization and domain decomposition techniques have significantly reduced simulation times for large 3D reservoirs (Sohrabi et al., 2019; Fowler et al., 2016). Hybrid CPU-GPU solvers also enable the integration of real-time monitoring data for continuous model updating (Demirer et al., 2023; Jiang et al., 2023).

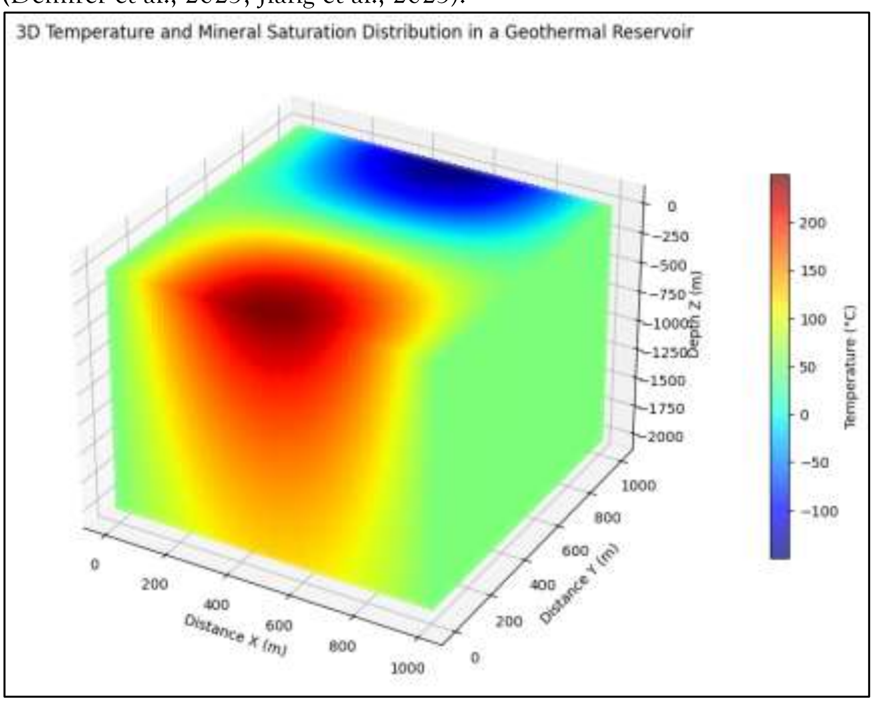

Figure 1: Example of 3D Temperature and Mineral Saturation Distribution in a Simulated Geothermal Reservoir

3.5 Hybrid and Reduced-Order Modelling

To address computational challenges, reduced-order models (ROMs) and hybrid approaches combining machine learning with physics-based RTM are increasingly applied (Mudunuru et al., 2017; Jiang et al., 2022). These methods approximate complex THC simulations with surrogate models that maintain accuracy while drastically lowering computational requirements. For example, recurrent neural networks have been used to predict thermal output and reservoir response based on historical simulation data, allowing for faster scenario testing and uncertainty quantification (Jiang et al., 2023; Demirer et al., 2023).

In sum, Numerical frameworks and modelling approaches in geothermal reactive transport provide a powerful methodology for predicting long-term reservoir performance. The integration of multi-physics coupling, high-performance computing, and hybrid machine learning techniques ensures accurate simulations of complex thermal, hydraulic, and geochemical interactions. Future developments should continue to focus on scalability, uncertainty quantification, and adaptive model calibration, thereby supporting sustainable and optimized geothermal resource exploitation (Aradóttir et al., 2012; Ma et al., 2023; Parisio et al., 2019).

4. Long-Term Performance and Sustainability Assessment

The long-term performance and sustainability of geothermal reservoirs are critical determinants of their economic viability and environmental acceptability. Sustained heat extraction inevitably perturbs the coupled thermal, hydraulic, and geochemical equilibrium of subsurface systems, leading to progressive changes in temperature distribution, fluid pathways, and mineralogical composition. Numerical modelling of reactive transport has therefore emerged as an essential tool for anticipating reservoir evolution over decadal timescales and for supporting adaptive reservoir management strategies. Unlike purely thermal or hydraulic models, reactive transport frameworks explicitly account for feedback mechanisms between fluid flow, heat transfer, and geochemical reactions, which are known to exert a decisive influence on long-term reservoir behavior (Bächler & Kohl, 2005; Alt-Epping & Diamond, 2008).

4.1 Conceptualizing Long-Term Geothermal Reservoir Performance

Long-term geothermal performance is commonly defined by the ability of a reservoir to maintain economically exploitable temperatures and flow rates under sustained production and reinjection. Numerical studies have demonstrated that thermal depletion alone does not fully explain observed declines in productivity; instead, permeability evolution driven by mineral dissolution and precipitation plays a central role (Blöcher et al., 2010; Kühn et al., 2002). Reactive transport models enable the explicit representation of these coupled processes, allowing performance metrics such as thermal drawdown, injectivity loss, and chemical scaling potential to be evaluated concurrently (Mottaghy et al., 2011; Sonney & Vuataz, 2009).

4.2 Sustainability Criteria and Indicators in Reactive Transport Modelling

Sustainability assessment within reactive transport frameworks relies on a suite of quantitative indicators that reflect both thermal longevity and reservoir integrity. These indicators typically include temperature recovery rates, porosity and permeability evolution, mineral saturation indices, and long-term mass balance of reactive species (Torresan et al., 2022; Bujakowski et al., 2016). Studies of sedimentary and fractured geothermal systems indicate that reservoirs may appear thermally sustainable while simultaneously undergoing geochemical degradation that compromises long-term productivity (García-Gil et al., 2016; Parisio et al., 2019).

Table 3: Key Sustainability Indicators in Reactive Transport Modelling of Geothermal Reservoirs

Indicator	What It Measures	Long-Term Implication	Representative Studies
Thermal Drawdown Rate	Rate of reservoir temperature decline	Controls productive lifetime of the reservoir	Blöcher et al.; Mottaghy et al.
Permeability Change	Evolution of flow capacity due to reactions	Affects injectivity and productivity	Kühn et al.; Bartels et al.
Dominant Reactions	Key dissolution–precipitation processes	Governs clogging or enhancement effects	Alt-Epping et al.; Ma et al.
Scaling Risk	Likelihood of mineral precipitation	Increases operational and maintenance costs	García-Gil et al.; Parisio et al.
Reinjection Effects	Thermal and chemical impacts of reinjection	Influences sustainability and thermal recovery	Torresan et al.; Kühn & Stöfen

4.3 Effects of Reinjection Strategies on Long-Term Reservoir Evolution

Reinjection plays a dual role in geothermal sustainability by supporting pressure maintenance while potentially accelerating thermal breakthrough and geochemical alteration. Reactive transport simulations have shown that reinjected fluids can induce localized cooling and trigger mineral precipitation reactions that reduce permeability near injection wells (Kühn & Stöfen, 2005; Alt-Epping et al., 2013). Long-term simulations further demonstrate that reinjection temperature, chemistry, and spatial configuration critically influence the balance between pressure support and thermal sustainability (Parisio et al., 2019; Torresan et al., 2022).

4.4 Porosity–Permeability Feedbacks and Reservoir Longevity

Porosity and permeability evolution represent one of the most significant uncertainties in long-term geothermal forecasting. Coupled reactive transport models have revealed non-linear feedbacks in which minor geochemical reactions can lead to disproportionate changes in flow pathways and heat extraction efficiency (Bartels et al., 2005; Fowler et al., 2016). In enhanced geothermal systems, chemical stimulation and prolonged circulation may initially improve permeability but eventually promote secondary mineral precipitation that limits long-term performance (Ma et al., 2023; Altar et al., 2023).

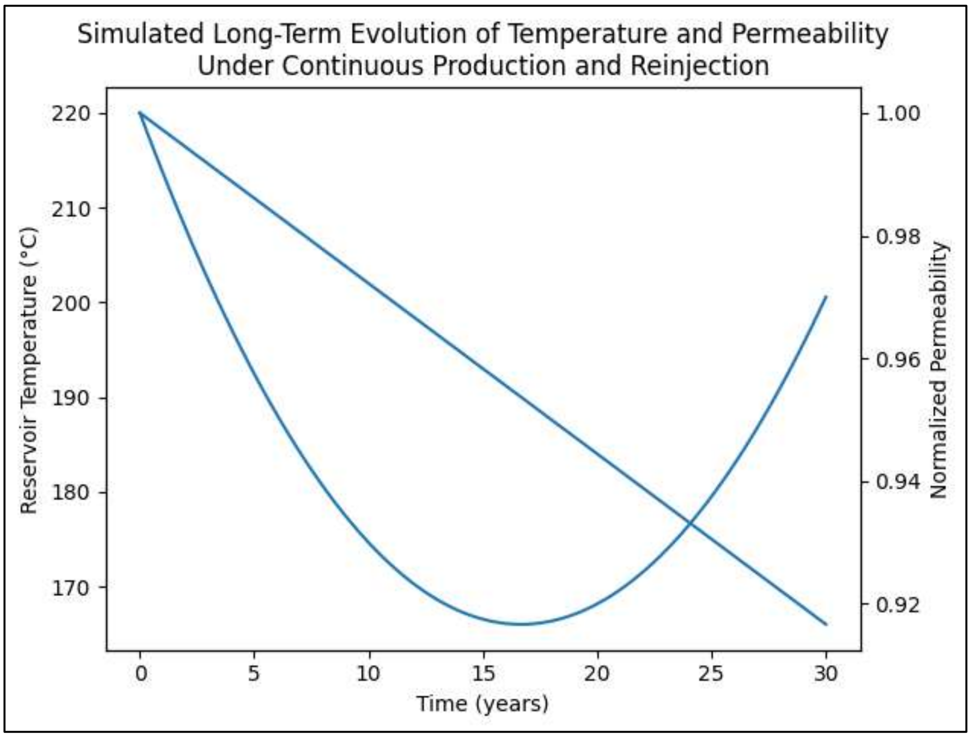

Figure 2: Simulated Long-Term Evolution of Temperature and Permeability in a Geothermal Reservoir.

4.5 Uncertainty and Sensitivity in Long-Term Performance Predictions

Despite advances in numerical techniques, long-term sustainability assessments remain subject to significant uncertainty due to limited subsurface characterization, scale effects, and parameter non-uniqueness. Sensitivity analyses consistently show that mineral reaction kinetics, fracture permeability, and fluid composition exert strong control on predicted reservoir evolution (Egert, 2021; Abd & Abushaikha, 2021). As a result, long-term predictions are increasingly framed probabilistically, with ensembles of reactive transport simulations used to bracket plausible performance trajectories (Erol et al., 2023).

4.6 Integration of Reduced-Order and Data-Driven Approaches

To overcome computational constraints associated with long-term reactive transport simulations, reduced-order and hybrid modelling approaches have gained prominence. Regression-based surrogate models and machine-learning-assisted frameworks enable rapid evaluation of long-term scenarios while preserving key system dynamics (Mudunuru et al., 2017; Demirer et al., 2023). In particular, recurrent neural network architectures trained on reactive transport outputs have demonstrated strong capability in forecasting long-term thermal and production trends across multiple operational scenarios (Jiang et al., 2022, 2023).

In sum, Long-term performance and sustainability assessment of geothermal reservoirs requires modelling frameworks capable of capturing the complex interplay between thermal, hydraulic, and geochemical processes. Reactive transport modelling provides a robust basis for evaluating reservoir longevity, identifying sustainability thresholds, and informing adaptive management strategies. While uncertainties remain, especially regarding permeability evolution and geochemical kinetics, recent methodological advances and hybrid modelling approaches significantly enhance predictive capability. As geothermal deployment expands, reactive transport-based sustainability assessment will remain indispensable for ensuring reliable, efficient, and responsible exploitation of subsurface heat resources.

5. Advances in Computational Techniques

The increasing complexity of geothermal reservoirs, characterized by tightly coupled thermal, hydraulic, mechanical, and geochemical processes, has driven significant advances in computational techniques for reactive transport modelling. Traditional numerical approaches, while physically robust, often struggle to resolve the multi-scale, non-linear interactions governing long-term reservoir evolution under sustained production and reinjection. Consequently, recent research has focused on improving numerical efficiency, scalability, and predictive capability through algorithmic innovations, high-performance computing, and hybrid modelling strategies. These advances have substantially expanded the applicability of reactive transport models from conceptual analyses to field-scale, long-term performance prediction in geothermal systems (Alt-Epping & Diamond, 2008; Fowler et al., 2016).

5.1 High-Resolution Spatial Discretization and Mesh Technologies

One of the most significant computational advances in reactive transport modelling has been the adoption of flexible spatial discretization techniques capable of capturing geological heterogeneity and complex flow pathways. Unstructured meshes, including finite-element and finite-volume formulations, allow for accurate representation of faults, fractures, and stratigraphic discontinuities that strongly influence geothermal fluid circulation (Fowler et al., 2016). These approaches have been shown to improve numerical stability and accuracy when simulating sharp thermal and chemical gradients near wells and reinjection zones (Blöcher et al., 2010).

Adaptive mesh refinement (AMR) techniques further enhance computational efficiency by dynamically increasing resolution in regions of high reactive activity, such as mineral precipitation fronts or thermal breakthrough zones, while maintaining coarser resolution elsewhere. Such methods reduce computational cost without compromising accuracy, making long-term reservoir simulations more tractable (Bartels et al., 2005; Bundschuh & Arriaga, 2010).

5.2 Coupled Multi-Physics and Fully Integrated THC Solvers

Modern geothermal simulators increasingly employ fully coupled thermal–hydraulic–chemical (THC) formulations rather than sequential or loosely coupled approaches. Fully integrated solvers simultaneously resolve flow, heat transport, and geochemical reactions, reducing numerical splitting errors and improving the representation of strong feedback mechanisms between permeability evolution and fluid chemistry (Bächler & Kohl, 2005; Kühn & Stöfen, 2005).

These solvers are particularly important for long-term performance prediction, where cumulative geochemical effects can significantly alter reservoir properties over decades of operation. Applications to sedimentary and volcanic geothermal systems demonstrate that coupled THC models outperform simplified approaches in predicting scaling, dissolution-induced porosity enhancement, and thermal drawdown patterns (Mottaghy et al., 2011; Torresan et al., 2022).

Table 4: Comparison of Numerical Discretization and Coupling Strategies in Geothermal Reactive Transport Modelling

Spatial Discretization Method	Coupling Approach	Computational Cost	Strengths	Limitations	Representative Geothermal Applications
Structured mesh (finite difference / finite volume)	Sequential (operator splitting)	Low to moderate	Simple implementation; computationally efficient for homogeneous reservoirs; suitable	Limited ability to represent complex geology; higher numerical errors for strongly	Conceptual and basin-scale geothermal models; early-stage reservoir assessments

			for preliminary assessments	coupled processes	
Structured mesh	Iterative coupling	Moderate	Improved accuracy over sequential schemes; better representation of feedbacks between flow, heat, and chemistry	Increased computational time; convergence issues in highly non-linear systems	Sedimentary geothermal reservoirs with moderate geochemical reactivity
Unstructured mesh (finite element / finite volume)	Sequential	Moderate	Flexible representation of faults, fractures, and irregular geometries; improved spatial accuracy	Operator splitting errors may persist; weaker feedback resolution	Fault-controlled geothermal systems; fractured reservoirs
Unstructured mesh	Fully coupled THC	High	High numerical accuracy; robust handling of strong thermal–hydraulic–chemical feedbacks; suitable for long-term prediction	Computationally intensive; requires high-performance computing resources	Enhanced geothermal systems (EGS); long-term sustainability and reinjection studies
Adaptive mesh refinement (AMR)	Fully coupled THC	High (optimized)	Dynamic resolution of reactive fronts and thermal gradients; efficient long-term simulations	Complex implementation; higher model setup effort	Reservoir-scale simulations with evolving permeability and mineral alteration

5.3 High-Performance Computing and GPU Acceleration

The computational intensity of reactive transport simulations has historically limited their application to simplified geometries or short time horizons. Recent advances in high-performance computing (HPC), including parallelization and graphics processing unit (GPU) acceleration, have significantly alleviated these constraints. GPU-based simulators enable massive parallel execution of transport and reaction calculations, reducing runtimes by orders of magnitude compared to conventional CPU-based implementations (Sohrabi et al., 2019).

Such platforms facilitate three-dimensional, field-scale simulations incorporating porosity and permeability evolution, thereby improving the reliability of long-term geothermal performance forecasts. HPC-enabled models have been successfully applied to enhanced geothermal systems and deep reservoirs, where fine temporal resolution is required to capture transient thermal and chemical dynamics (Parisio et al., 2019; Kühn et al., 2002).

5.4 Reduced-Order Modelling and Surrogate Techniques

Despite advances in computational power, full-scale reactive transport models remain computationally expensive for uncertainty analysis, optimization, and real-time decision support. Reduced-order models (ROMs) have emerged as an effective solution by approximating the behavior of high-fidelity simulations using regression, projection, or statistical learning techniques (Mudunuru et al., 2017).

ROMs trained on detailed numerical simulations can rapidly predict key performance indicators such as thermal output, pressure evolution, and mineral alteration trends. These approaches are particularly valuable for scenario analysis and long-term forecasting under varying production strategies, enabling efficient exploration of operational uncertainty while preserving essential physical behavior (Demirer et al., 2023).

Title 4: Emerging Computational Techniques for Long-Term Geothermal Reactive Transport Simulation

Technique	Primary Objective	Typical Computational Savings	Key Limitations	Representative Studies and Applications
High-Performance Computing (HPC)	Enable large-scale, high-resolution 3D reactive transport simulations over long time horizons	One to two orders of magnitude reduction in wall-clock time through parallelization	Requires access to advanced computing infrastructure; increased model complexity	Field-scale geothermal reservoir simulations with coupled THC processes (Parisio et al.; Torresan et al.)
GPU Acceleration	Accelerate transport and reaction calculations via massive parallel processing	Up to two orders of magnitude speed-up compared to CPU-only implementations	Limited portability; algorithm restructuring required; memory constraints	GPU-based reactive transport simulators for EGS and deep geothermal systems (Sohrabi et al.)
Reduced-Order Models (ROMs)	Rapid approximation of high-fidelity model outputs for forecasting and scenario analysis	Several orders of magnitude reduction after training	Loss of fine-scale physical detail; dependence on training data quality	Long-term thermal output prediction and uncertainty analysis in geothermal systems (Mudunuru et al.)
Machine Learning Surrogates	Capture non-linear system behavior for fast prediction of reservoir performance metrics	Orders of magnitude reduction during inference	Limited interpretability; risk of extrapolation errors	Energy production and temperature forecasting using recurrent neural networks (Jiang et al.)
Hybrid Physics–Data Models	Combine physical consistency with computational efficiency	Significant runtime reduction while preserving interpretability	Integration complexity; data and calibration requirements	Coupled ML–RTM frameworks for long-term geothermal performance prediction (Demirer et al.)

5.5 Integration of Machine Learning with Physics-Based Models

Hybrid modelling frameworks combining machine learning with physics-based reactive transport simulations represent a rapidly growing research direction. Recurrent neural networks and multiscale learning architectures have demonstrated strong capability in capturing temporal dependencies and non-linear reservoir behavior when trained on numerical simulation outputs (Jiang et al., 2022).

Recent developments emphasize physics-informed and data-assisted learning approaches, where machine learning models complement rather than replace mechanistic simulators. Such integration enhances predictive accuracy while maintaining physical interpretability, particularly for long-term energy production forecasting and reservoir management applications (Jiang et al., 2023).

5.6 Uncertainty Quantification and Model Scalability

Advances in computational techniques have also improved the treatment of uncertainty in geothermal reactive transport modelling. Parallel computing and surrogate models enable large ensemble simulations, supporting probabilistic assessment of reservoir performance under uncertain geological, hydraulic, and geochemical parameters (Egert, 2021). These developments are critical for risk-informed decision-making and for evaluating the robustness of long-term production strategies (Erol et al., 2023).

Overall, Advances in computational techniques have fundamentally transformed reactive transport modelling into a practical and powerful tool for long-term geothermal reservoir performance prediction. Innovations in spatial discretization, coupled multi-physics solvers, high-performance computing, and hybrid data-driven approaches have significantly enhanced model accuracy, scalability, and applicability. While challenges related to uncertainty, data availability, and computational demand persist, ongoing methodological developments continue to narrow the gap between numerical prediction and field-scale geothermal management, reinforcing the role of advanced computational modelling in sustainable geothermal energy exploitation.

6. Hybrid and Data-Driven Modelling Strategies

The increasing complexity of geothermal reservoirs, coupled with the long temporal horizons required for performance prediction, has exposed the computational and practical limitations of purely physics-based reactive transport models. While high-fidelity numerical simulators are indispensable for capturing coupled thermal, hydraulic, mechanical, and geochemical processes, their application to long-term forecasting, uncertainty analysis, and real-time decision support remains constrained by high computational cost and parameter uncertainty (Blöcher et al., 2010; Fowler et al., 2016). In response, hybrid and data-driven modelling strategies have emerged as a complementary paradigm, integrating machine learning, reduced-order modelling, and statistical inference with physics-based reactive transport frameworks. These approaches aim to preserve physical consistency while enhancing predictive efficiency, scalability, and adaptability for long-term geothermal reservoir management.

6.1 Motivation for Hybrid Modelling in Reactive Transport Simulations

Reactive transport modelling in geothermal systems involves solving highly nonlinear, tightly coupled partial differential equations governing fluid flow, heat transport, and geochemical reactions. Such models are particularly sensitive to spatial heterogeneity, evolving porosity–permeability relationships, and poorly constrained kinetic parameters (Alt-Epping & Diamond, 2008; Kühn & Stöfen, 2005). When applied to field-scale systems over decadal timeframes, these complexities often lead to prohibitive runtimes and limited feasibility for ensemble-based uncertainty quantification or optimization studies (Sohrabi et al., 2019).

Hybrid modelling strategies address these challenges by combining physics-based simulations with data-driven components that act as surrogates, emulators, or corrective layers. This integration enables rapid evaluation of system responses while retaining essential physical constraints, making hybrid models particularly suitable for long-term performance prediction under multiple operational scenarios (Mudunuru et al., 2017; Torresan et al., 2022).

6.2 Reduced-Order Models for Long-Term Performance Prediction

Reduced-order models (ROMs) constitute one of the earliest and most widely adopted hybrid approaches in geothermal modelling. ROMs aim to approximate the behaviour of high-fidelity reactive transport simulations using a lower-dimensional representation derived from regression, proper orthogonal decomposition, or response surface methodologies (Mudunuru et al., 2017). These models are typically trained on outputs from detailed numerical simulations and are capable of reproducing transient thermal output and production trends with substantially reduced computational effort.

In geothermal applications, ROMs have demonstrated strong potential for predicting long-term thermal decline, evaluating reinjection strategies, and supporting operational decision-making in enhanced geothermal systems (EGS) (Bächler & Kohl, 2005; Mudunuru et al., 2017). However, their accuracy is strongly dependent on the representativeness of the training dataset and their ability to capture nonlinear geochemical feedbacks remains limited when extrapolated beyond calibrated conditions.

6.3 Machine Learning Techniques in Geothermal Reservoir Modelling

Recent advances in machine learning have significantly expanded the scope of data-driven modelling in geothermal systems. Artificial neural networks (ANNs), recurrent neural networks (RNNs), and deep learning architectures have been applied to predict reservoir pressure, temperature evolution, and energy production based on historical simulation or field data (Jiang et al., 2022; Demirer et al., 2023).

RNN-based approaches are particularly well suited for geothermal applications due to their ability to capture temporal dependencies and long-term system memory. Studies have shown that multiscale RNN frameworks can successfully reproduce both short-term dynamics and long-term production trends when trained on numerical simulation outputs, offering a computationally efficient alternative to repeated reactive transport simulations (Jiang et al., 2022, 2023). Importantly, these models enable rapid scenario testing and sensitivity analysis, which are critical for long-term reservoir management.

6.4 Hybrid Physics–Machine Learning Frameworks

Beyond standalone data-driven models, hybrid physics–machine learning frameworks explicitly embed physical knowledge into learning architectures. In such approaches, machine learning models are constrained by governing equations, conservation laws, or physics-based residuals, thereby improving interpretability and robustness (Demirer et al., 2023). For reactive transport applications, hybrid frameworks have been used to accelerate geochemical reaction calculations, approximate constitutive relationships, or emulate computationally intensive sub-processes such as mineral precipitation and dissolution kinetics.

In geothermal reservoirs, these hybrid methods have been shown to enhance the efficiency of reactive transport simulations without sacrificing physical realism, particularly in systems where geochemical reactions strongly influence porosity and permeability evolution (Ma et al., 2023; Alt-Epping et al., 2013). By selectively replacing high-cost components of numerical simulators, hybrid frameworks enable long-term forecasting at spatial and temporal scales previously unattainable.

6.5 Data Assimilation, Uncertainty Quantification, and Model Updating

Hybrid and data-driven models also play a critical role in uncertainty quantification and data assimilation. Long-term geothermal predictions are inherently uncertain due to limited subsurface characterization, scale effects, and evolving reservoir conditions (Egert, 2021; Abd & Abushaikha, 2021). Data-driven surrogates allow for efficient ensemble simulations, enabling probabilistic assessment of reservoir performance under varying geological and operational assumptions.

Moreover, machine learning models can be continuously updated as new production and monitoring data become available, facilitating adaptive reservoir management. This capability is particularly valuable for geothermal systems subject to chemical stimulation, reinjection-induced cooling, or geochemical alteration over time (Erol et al., 2023; García-Gil et al., 2016).

6.6 Limitations and Challenges of Hybrid Approaches

Despite their advantages, hybrid and data-driven modelling strategies are not without limitations. Machine learning models often suffer from limited extrapolation capability and may produce physically inconsistent predictions when applied outside their training domain (Jiang et al., 2023). Furthermore, the integration of data-driven components into reactive transport frameworks requires careful validation to ensure that critical geochemical feedbacks and long-term degradation mechanisms are not overlooked (Parisio et al., 2019).

Another key challenge lies in data availability and quality. High-resolution datasets suitable for training robust machine learning models remain scarce for many geothermal fields, particularly during early development stages (Blöcher et al., 2010; Torresan et al., 2022).

In sum, Hybrid and data-driven modelling strategies represent a significant advancement in the numerical modelling of reactive transport in geothermal reservoirs. By combining the physical rigor of traditional reactive transport simulations with the efficiency and adaptability of machine learning and reduced-order models, these approaches offer a powerful framework for long-term performance prediction. While challenges related to data availability, model generalization, and physical interpretability remain, ongoing methodological developments suggest that hybrid modelling will play an increasingly central role in sustainable geothermal reservoir management.

7. Applications and Case Studies

Reactive transport modelling (RTM) has become an indispensable tool for evaluating the long-term behavior and performance of geothermal reservoirs under operational conditions. By explicitly coupling fluid flow, heat transport, and geochemical reactions, RTM enables a more realistic representation of reservoir evolution than purely thermal–hydraulic models. This section reviews key applications and representative case studies where numerical reactive transport models have been applied to assess sustainability, predict production decline, evaluate chemical stimulation strategies, and manage geochemical risks in both conventional and enhanced geothermal systems.

7.1 Conventional Hydrothermal Geothermal Reservoirs

Reactive transport modelling has been extensively applied to conventional hydrothermal geothermal systems to understand temperature evolution, mineral alteration, and permeability changes during prolonged exploitation. Early three-dimensional numerical studies demonstrated that fluid–rock interactions can significantly modify reservoir properties over time, thereby influencing heat recovery efficiency and production lifespan (Blöcher et al., 2010; Mottaghy et al., 2011).

Well-documented case studies include the geothermal projects at Den Haag in the Netherlands and Bad Blumau in Austria, where RTM was used to simulate temperature evolution, scaling risks, and the coupled extraction of heat and dissolved gases (Mottaghy et al., 2011; Alt-Epping et al., 2013). These studies highlighted that mineral precipitation and dissolution processes may either enhance or impair reservoir permeability depending on local thermodynamic and hydrodynamic conditions. Similarly, long-term simulations of Alpine geothermal systems have shown that reactive transport effects must be considered to avoid overestimating sustainable production rates (Sonney & Vuataz, 2009).

7.2 Long-Term Sustainability and Renewability Assessment

One of the most critical applications of RTM lies in evaluating the long-term sustainability and renewability of geothermal reservoirs under continuous production and reinjection. Numerical models incorporating geochemical reactions have been used to assess whether reinjected fluids induce adverse mineralogical changes that may compromise reservoir performance (Torresan et al., 2022; Bujakowski et al., 2016).

The Podhale geothermal reservoir in Poland provides a representative example where coupled flow–heat–chemistry simulations were applied to forecast production behavior over several decades (Bujakowski et al., 2016). Results demonstrated that reactive processes influence both thermal breakthrough and permeability evolution, reinforcing the importance of integrating RTM into reservoir management strategies. Comparable findings were reported for sedimentary geothermal systems, where chemical reactions within porous media were shown to affect reservoir quality and long-term heat extraction efficiency (Xiao & Jones, 2018; Moore, 2020).

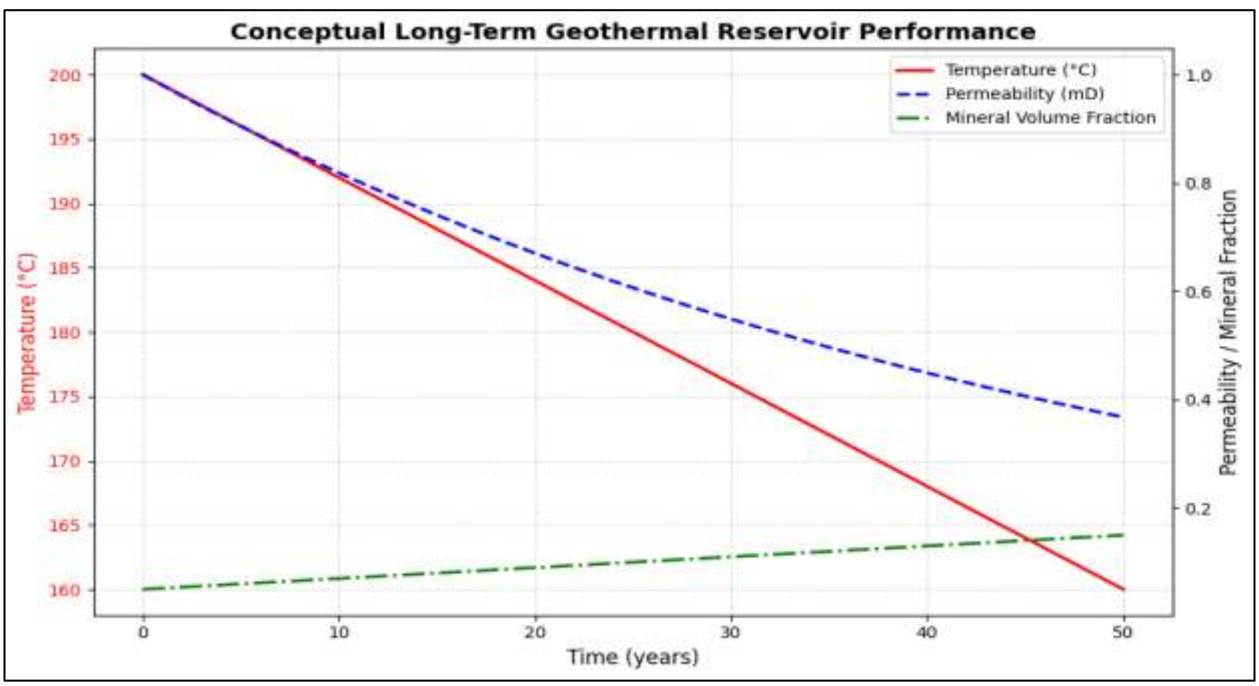

Figure 3: Long-Term Evolution of Temperature, Permeability, and Mineral Volume Fraction in a Geothermal Reservoir under Sustained Production and Reinjection

7.3 Enhanced Geothermal Systems and Chemical Stimulation

Reactive transport modelling plays a particularly prominent role in enhanced geothermal systems (EGS), where artificial stimulation and fluid injection intentionally alter reservoir properties. Coupled thermal–hydraulic–chemical models have been used to simulate the impact of chemical stimulation on fracture permeability and mineral dissolution–precipitation dynamics (Bächler & Kohl, 2005; Ma et al., 2023).

Recent studies demonstrate that RTM can predict unintended consequences of stimulation, such as secondary mineral precipitation that reduces permeability gains over time (Ma et al., 2023). Field-scale applications emphasize that ignoring reactive processes may result in overly optimistic predictions of stimulation effectiveness. Numerical investigations of EGS reservoirs further show that permeability evolution is highly sensitive to fluid composition, temperature gradients, and reaction kinetics (Kühn et al., 2002; Bartels et al., 2005).

7.4 CO_2-Rich and Reactive Fluid Geothermal Systems

Reactive transport modelling has also been applied to geothermal systems involving CO_2-rich fluids or coupled geothermal–carbon management scenarios. Multidimensional simulations of basalt-hosted geothermal reservoirs have demonstrated the potential for mineral carbonation to permanently trap CO_2 while simultaneously influencing porosity and permeability evolution (Aradóttir et al., 2012).

Studies investigating CO_2 migration through fractured and faulted geothermal formations highlight the importance of reactive transport processes in controlling long-term fluid pathways and reservoir integrity (Marín-Moreno et al., 2019). Furthermore, RTM has been used to assess the geochemical alteration of wellbore materials and surrounding formations, providing insights into long-term operational risks associated with reactive fluids (Gherardi et al., 2012).

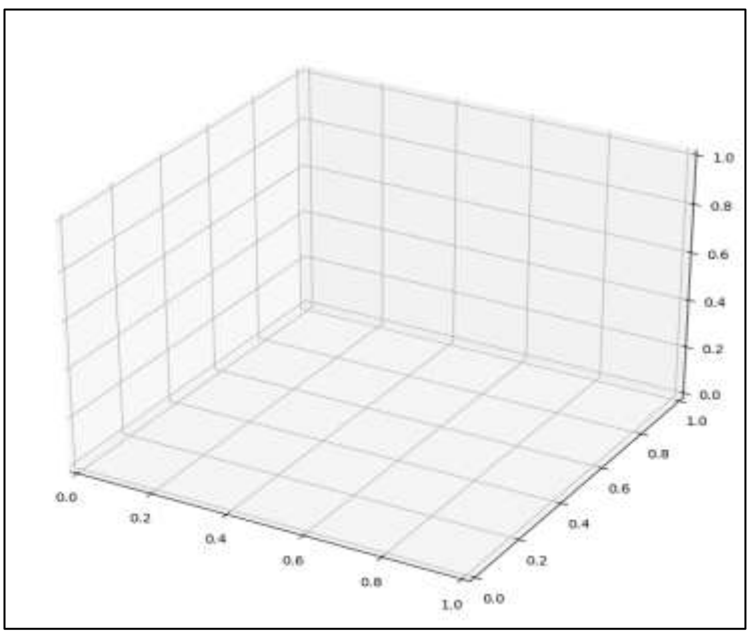

Figure 4: 3D Schematic of Reactive Transport Processes in a Geothermal Reservoir

7.5 Integration of Machine Learning and Reduced-Order Models

Due to the computational intensity of fully coupled reactive transport simulations, recent applications increasingly combine RTM with reduced-order and machine learning approaches. Regression-based reduced-order models have been successfully employed to approximate transient thermal output and reservoir behavior with significantly reduced computational cost (Mudunuru et al., 2017).

More recently, recurrent neural networks and multiscale learning frameworks have been trained on RTM-generated datasets to predict short- and long-term geothermal energy production (Jiang et al., 2022, 2023). Hybrid approaches that integrate physics-based constraints with data-driven models offer promising pathways for real-time forecasting and decision support while preserving the physical interpretability of numerical simulations (Demirer et al., 2023).

8. CONCLUSION: CHALLENGES, UNCERTAINTIES, AND FUTURE DIRECTIONS

Despite significant advances in numerical modelling of reactive transport in geothermal reservoirs, several challenges and sources of uncertainty continue to limit the predictive accuracy of long-term performance assessments. One of the primary difficulties lies in the inherent complexity of coupling thermal, hydraulic, and geochemical processes across multiple spatial and temporal scales. Reaction kinetics, mineral surface areas, and thermodynamic parameters are often poorly constrained, leading to uncertainties in predicting porosity and permeability evolution over extended operational periods.

Additional uncertainty arises from the limited availability of high-resolution field data for model calibration and validation. Subsurface heterogeneity, fracture network complexity, and evolving reservoir conditions introduce scale-dependent effects that are difficult to capture using conventional continuum-based approaches. As a result, model outcomes remain sensitive to assumptions regarding reservoir structure, boundary conditions, and fluid–rock interaction mechanisms.

From a computational perspective, fully coupled three-dimensional reactive transport simulations remain resource-intensive, restricting their routine application in real-time reservoir management. While recent progress in high-performance computing and numerical solvers has improved model efficiency, the trade-off between physical realism and computational feasibility persists, particularly for field-scale and long-term simulations.

Future research directions should focus on integrating physics-based reactive transport models with data-driven and reduced-order approaches to enhance computational efficiency without compromising physical consistency. Hybrid modelling frameworks, incorporating machine learning and adaptive parameter updating, offer promising pathways for uncertainty reduction and real-time forecasting. Moreover, improved field monitoring techniques, including geochemical tracers and time-lapse observations, are essential for constraining model parameters and validating predictions.

Ultimately, advancing the reliability of reactive transport modelling for geothermal applications will require closer integration between numerical modelling, laboratory experimentation, and field-scale observations. Addressing these challenges will strengthen the role of reactive transport models as robust decision-support tools for sustainable geothermal reservoir development and long-term energy production.

REFERENCES

1. Blöcher, M. G., Zimmermann, G., Moeck, I., Brandt, W., Hassanzadegan, A., & Magri, F. (2010). 3D numerical modeling of hydrothermal processes during the lifetime of a deep geothermal reservoir. Geofluids, 10(3), 406-421.
2. Jiang, A., Qin, Z., Faulder, D., Cladouhos, T. T., & Jafarpour, B. (2022). Recurrent neural networks for short-term and long-term prediction of geothermal reservoirs. Geothermics, 104, 102439.
3. Mottaghy, D., Pechnig, R., & Vogt, C. (2011). The geothermal project Den Haag: 3D numerical models for temperature prediction and reservoir simulation. Geothermics, 40(3), 199-210.
4. Demirer, E., Coene, E., Iraola, A., Nardi, A., Abarca, E., Idiart, A., ... & Rodríguez-Morillas, N. (2023). Improving the performance of reactive transport simulations using artificial neural networks. Transport in Porous Media, 149(1), 271-297.
5. Mudunuru, M. K., Karra, S., Harp, D. R., Guthrie, G. D., & Viswanathan, H. S. (2017). Regression-based reduced-order models to predict transient thermal output for enhanced geothermal systems. Geothermics, 70, 192-205.
6. Aradóttir, E. S. P., Sonnenthal, E. L., Björnsson, G., & Jónsson, H. (2012). Multidimensional reactive transport modeling of CO2 mineral sequestration in basalts at the Hellisheidi geothermal field, Iceland. International Journal of Greenhouse Gas Control, 9, 24-40.
7. Alt-Epping, P., & Diamond, L. W. (2008). Reactive transport and numerical modeling of seafloor hydrothermal systems: a review. Magma to Microbe: modeling hydrothermal processes at ocean spreading centers, 178, 167-192.
8. Xiao, Y., & Jones, G. D. (2018). Reactive transport modeling and reservoir quality prediction. Reactive transport modeling: Applications in subsurface energy and environmental problems, 157-235.
9. Ma, L., Cui, Z., Feng, B., Qi, X., Zhao, Y., & Zhang, C. (2023). Reactive transport modeling of chemical stimulation processes for an enhanced geothermal system (EGS). Energies, 16(17), 6229.
10. Abd, A. S., & Abushaikha, A. S. (2021). Reactive transport in porous media: a review of recent mathematical efforts in modeling geochemical reactions in petroleum subsurface reservoirs. SN Applied Sciences, 3(4), 401.
11. Alt-Epping, P., Waber, H. N., Diamond, L. W., & Eichinger, L. (2013). Reactive transport modeling of the geothermal system at Bad Blumau, Austria: Implications of the combined extraction of heat and CO2. Geothermics, 45, 18-30.
12. Torresan, F., Piccinini, L., Cacace, M., Pola, M., Zampieri, D., & Fabbri, P. (2022). Numerical modeling as a tool for evaluating the renewability of geothermal resources: the case study of the Euganean Geothermal System (NE Italy). Environmental geochemistry and health, 44(7), 2135-2162.
13. Altar, D. E., Zarrouk, S., & Kaya, E. (2023, November). Understanding Mineralogical and Geochemical Evolution in Geothermal Reservoirs through Reactive Transport Modelling. In Proceedings 45th New Zealand Geothermal Workshop (Vol. 15, p. 17).

14. Kühn, M., Bartels, J., & Iffland, J. (2002). Predicting reservoir property trends under heat exploitation: interaction between flow, heat transfer, transport, and chemical reactions in a deep aquifer at Stralsund, Germany. Geothermics, 31(6), 725-749.
15. Moore, K. R. (2020). Numerical reactive transport modeling of soluble mineral and fluid interactions in the subsurface and application to sedimentary geothermal systems.
16. Bächler, D., & Kohl, T. (2005). Coupled thermal–hydraulic–chemical modelling of enhanced geothermal systems. Geophysical Journal International, 161(2), 533-548.
17. Sohrabi, R., Omlin, S., & Miller, S. A. (2019). GEYSER: 3D thermo-hydrodynamic reactive transport numerical simulator including porosity and permeability evolution using GPU clusters. Computational Geosciences, 23(6), 1317-1330.
18. Jiang, A., Qin, Z., Faulder, D., Cladouhos, T. T., & Jafarpour, B. (2023). A multiscale recurrent neural network model for predicting energy production from geothermal reservoirs. Geothermics, 110, 102643.
19. Kühn, M., & Stöfen, H. (2005). A reactive flow model of the geothermal reservoir Waiwera, New Zealand. Hydrogeology Journal, 13(4), 606-626.
20. Sonney, R., & Vuataz, F. D. (2009). Numerical modelling of Alpine deep flow systems: A management and prediction tool for an exploited geothermal reservoir (Lavey-les-Bains, Switzerland). Hydrogeology Journal, 17(3), 601-616.
21. Bujakowski, W., Tomaszewska, B., & Miecznik, M. (2016). The Podhale geothermal reservoir simulation for long-term sustainable production. Renewable Energy, 99, 420-430.
22. Marín-Moreno, H., Bull, J. M., Matter, J. M., Sanderson, D. J., & Roche, B. J. (2019). Reactive transport modelling insights into CO2 migration through sub-vertical fluid flow structures. International Journal of Greenhouse Gas Control, 86, 82-92.
23. Egert, R. (2021). Flow and transport in fractured geothermal reservoirs on different scales: Linking experiments and numerical models (Doctoral dissertation, Karlsruher Institut für Technologie (KIT)).
24. Gherardi, F., Audigane, P., & Gaucher, E. C. (2012). Predicting long-term geochemical alteration of wellbore cement in a generic geological CO2 confinement site: Tackling a difficult reactive transport modeling challenge. Journal of Hydrology, 420, 340-359.
25. García-Gil, A., Epting, J., Ayora, C., Garrido, E., Vázquez-Suñé, E., Huggenberger, P., & Gimenez, A. C. (2016). A reactive transport model for the quantification of risks induced by groundwater heat pump systems in urban aquifers. Journal of Hydrology, 542, 719-730.
26. Fowler, S. J., Kosakowski, G., Driesner, T., Kulik, D. A., Wagner, T., Wilhelm, S., & Masset, O. (2016). Numerical simulation of reactive fluid flow on unstructured meshes. Transport in Porous Media, 112(1), 283-312.
27. Bundschuh, J., & Arriaga, M. S. (2010). Introduction to the numerical modeling of groundwater and geothermal systems. Introduction to the Numerical Modeling of Groundwater and Geothermal Systems, 217-284.
28. Bartels, J., Clauser, C., Kühn, M., Pape, H., & Schneider, W. (2005). Reactive flow and permeability prediction—numerical simulation of complex hydrogeothermal problems.
29. Parisio, F., Vilarrasa, V., Wang, W., Kolditz, O., & Nagel, T. (2019). The risks of long-term re-injection in supercritical geothermal systems. Nature communications, 10(1), 4391.
30. Erol, S., Akin, T., & Akin, S. (2023). Update for reactive transport modeling of the Kızıldere geothermal field to reduce uncertainties in the early inspections. Turkish Journal of Earth Sciences, 32(4), 541-554.