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Invited Commentary

REGIONAL SCALE SUBSURFACE MODELING

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ABSTRACT

The subsurface is a critical foundation for society, providing essential resources such as water, minerals, and energy, while also offering storage capacity for resources and waste. Current subsurface use is expanding rapidly, leading to aggregated effects at regional scales ranging from tens to hundreds of kilometers. Despite their growing importance, current subsurface models remain limited to field-scale analysis and are insufficient for understanding regional scale impacts. This commentary advocates for a shift in subsurface modeling research, highlighting the importance of developing regional scale models that can assess the cumulative and interconnected effects of multiple subsurface operations. We outline a roadmap for developing the mathematical and numerical foundations necessary for regional scale subsurface analysis, highlighting the need for multiscale modeling, hybrid physics- and data-driven modeling approaches, and efficient computational tools.

KEYWORDS

Geological, Subsurface, Resources

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1. THE SUBSURFACE IS THE FOUNDATION FOR SOCIETY

The subsurface is the source of resources as disparate as drinking water, critical minerals, and energy, while simultaneously providing seasonal to semi-permanent storage capacity for resources and waste. Demand for this multifunctional capacity is rapidly increasing, resulting in a transition from a past where subsurface resources were relatively abundant and scarcely exploited to a future where subsurface resources are constrained and densely exploited. With this transition necessarily comes a transition in the modeling paradigm, from where subsurface resources could be adequately modeled in isolation at a *field scale* (denoting herein the scale of a single industrial subsurface operation, typically on the order of a few kilometers horizontal extent) towards interacting systems at the *regional scale* (denoting here a scale of compound impact of a suite of subsurface operations, on the order of 10s to 100s of kilometers horizontal extent).

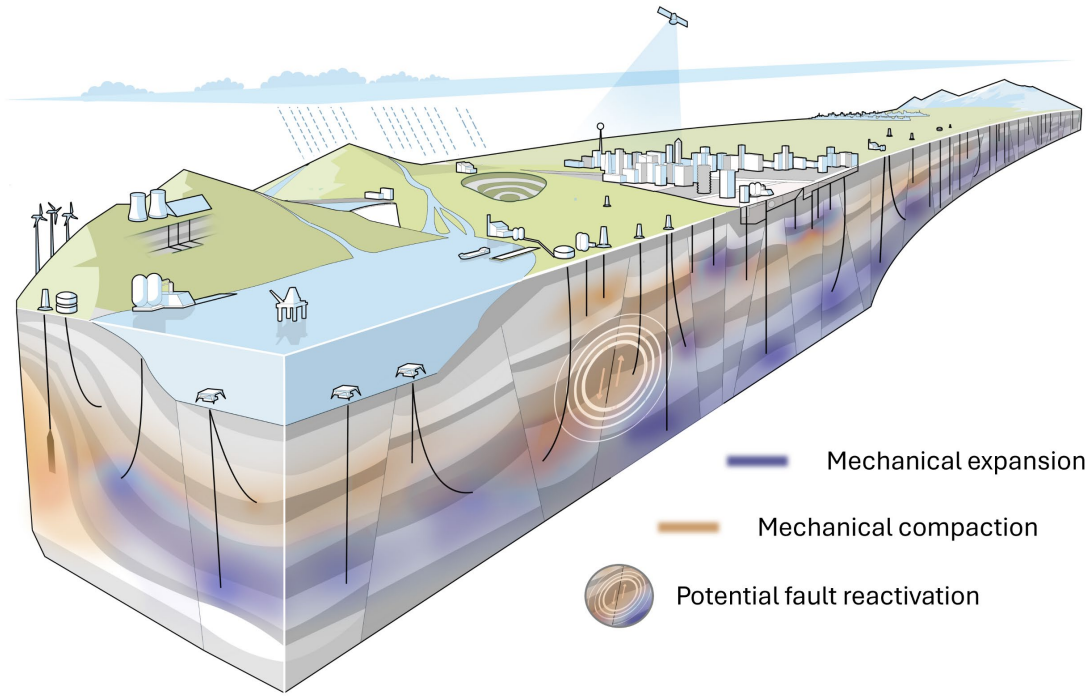


Figure 1: Conceptual illustration of regional scale subsurface activities and interactions.

Figure 1 summarizes some of these multifunctional uses of the subsurface, while at the same time qualitatively indicating the regional scale impact such use may have in terms of mechanical response. Importantly, while any individual subsurface operation may be benign, their interactions may critically interfere with both each other, as well as natural features in near-critical states.

The compound effect of multiple subsurface operations has already been appreciated in several instances. As motivation, we will review three paradigmatic examples. First, it is now generally known that excessive local groundwater extraction has led to a reduction in the groundwater levels. For example, in the North China Plain, groundwater levels are falling by around a meter per year over a region covering several hundred kilometers. This represents a regional scale change in the state of the subsurface, impacting both the land surface elevation, but also the mechanical state of the near-surface crust. Managing the causes and consequences of regional scale groundwater depletion is a multifaceted problem, necessarily relying on regional scale analysis tools (7).

As a second example, fluid injection has been linked to a peak in seismicity in the US midcontinent. In Oklahoma during the period from 2009 to 2019, high-rate wastewater injection wells have been associated with more than 2000 earthquakes greater than magnitude 3 (6, 13). This included the magnitude 5.6 Prague earthquake in 2011 and the magnitude 5.8 Pawnee earthquake in 2016, both of which caused significant damage (5). These earthquakes have been attributed to hydraulic fault reactivation caused by pressure build-up in faults, as well as poroelastically induced solid stress transfer triggering of moderate earthquakes more than 40 km from the wastewater injection wells (3). A similar experience of induced earthquakes was caused by gas extraction from the Groningen field, the largest gas field in Europe. Since the 1980s, hundreds of earthquakes have occurred due to the build-up of shear stresses on the numerous faults within the formation due to differences in compaction on either side of the faults. The induced earthquakes eventually led to further production being deemed unsafe. In 2023, normal gas production at the Groningen field ceased after 60 years of production, and it has been permanently closed from the 1st of October 2024 following a Dutch Senate ruling.

Finally, we mention the emerging situation in the North Sea, where geological CO_2 storage is being developed in close proximity to existing oil and gas production. Bottom-hole pressure measurements indicate strong pressure connectivity between different licenses, explicitly pointing to the fact that the system must be managed holistically across both different operators and across different subsurface resource usages.

These paradigmatic examples provide several key insights: i) subsurface resource utilization can cause destabilization of geological features such as faults at great distances from the operation itself; ii) the effects of resource utilization aggregates, possibly non-linearly, such that analysis is necessary at length- and time-scales beyond the field scale; iii) the impacts of subsurface operations may appear both as consequences to society (earthquakes, groundwater depletion, and subsidence), but also as an operational and economical consequence for other subsurface resources in the same region.

The aggregate regional scale consequences of industrial exploitation of the subsurface have thus been established. This Invited Commentary argues that this represents only the early stages of a much broader development, given the societal plans for future expansion of subsurface use. These can be illustrated by considering current and projected quantities of non-renewable subsurface withdrawal:

- Groundwater is already vital in meeting the rising water demands across multiple sectors. A further substantial increase is projected, reaching an estimated global peak with an annual global non-renewable withdrawal rate of 625 km^3 per year in 2050 (8). This represents an approximate doubling of the withdrawal rate since 2010.
- Many climate mitigation measures use water (10). Demand depends directly on the extent and type of climate mitigation that is realized, and may accumulate to 1000s of km^3 per year.
- To limit anthropogenic warming to 1.5°C, oil and gas production must likely decline by 3% every year in the period from 2021 to 2050. However, except for periods of global economic crises, such as those in the late 2000s and 2020, oil production has steadily increased each year over the past two decades, and in 2024, 5.8 km^3 were produced. Global natural gas production amounted to more than 4000 standard km^3 in 2024, equivalent to tens of km^3 at subsurface conditions (11).
- At the same time, the injection of fluid into the subsurface in the form of acid gas, CO_2 or wastewater is also projected to increase: Limiting anthropogenic warming to 1.5°C could require gigatons of CO_2 stored per year by 2050, compared to today's 30 Mt of CO_2 per year (4)
- Seasonal storage of thermal energy and gas will increase due to the energy transition.

While the quantification of each subsurface engineering operation listed above remains uncertain, the total and unbalanced production and injection of fluid will increase significantly as the use of the subsurface technology diversifies and expands.

A key problem which arises in this operational environment is the relative balance between short-term capacity and the sustainable long-term capacity of a subsurface resource, and that this balance cannot be understood for any resource in isolation, without an understanding of the development of the entire system on a regional scale.

These various uses of the subsurface, both over time and across adjacent regions, can interact in ways that create broader impacts than if each activity occurred in isolation. Importantly, our past and current use of the subsurface has consequences for how it can be used in the future.

We understand that already in the present, and inescapably in the future, regional scale interactions between a heterogeneous assembly of competing uses of subsurface resources need to be analyzed. Such analysis can no longer be conducted as an ad hoc response to observed regional scale impact but must become part of the routine planning and management for equitable use of subsurface resources. However, due to relatively little attention being afforded to regional scale subsurface issues in the past,

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a community with expertise and computational tools needed for such regional scale analysis does not exist. In the following, we detail a roadmap for developing such regional scale subsurface modeling and simulation capabilities.

2. CHALLENGES IN REGIONAL SCALE MODELING AND SIMULATION

Regional scale modeling naturally builds on the knowledge and methods developed for the field scale. However, as the scale of the problem changes, several new challenges arise. Some of the most critical are discussed in the following, including data availability and integration, modeling concepts, computational aspects, and our expectations as to the resulting forecasting skill.

2.1. The Interplay Between Modeling and Data

Quantitative modeling is inherently limited by the availability of accessible data. Here, the regional scale strongly deviates from the field scale.

From the geological perspective, it is reasonable to expect that with the increase in modeling scale, accompanied by a change in emphasis in the dominating physical processes, there is also an increase in the "necessary parameter resolution scale". Thus, while field scale simulations are inherently challenged by geological features at or below the resolution of seismic imaging, there is reason to be hopeful that the most important features needed for regional scale modeling are characterizable by seismic imaging if such data has been collected and is available.

On the other hand, from the anthropogenic perspective, regional scale data regarding human activities is not generally available. This can be clearly understood since at the field scale, the relevant human activities will be readily available within the operating entity. However, as this data may, to some extent, be confidential, it will commonly not be fully accessible through public databases. Moreover, the data that is publicly available may be heterogeneous, in the sense that the reporting requirements related to subsurface operations may not be uniform across a regional scale model.

Efforts to aggregate regional scale data are ongoing through collaborative initiatives such as the European Geological Data Infrastructure (EGDI) and EPOS (European Plate Observing System), and through efforts of the US Geological Survey. However, these databases are still incomplete, and in many instances, data may be available in different formats and with different conceptualization of their reliability, making direct use of the data difficult.

At the regional scale, geophysical data not commonly associated with field-scale operations may also become relevant. Examples include gravimetry, magnetotellurics, interferometric synthetic aperture radar (InSAR) and GPS for surface deformation and micro-seismic monitoring of pressure changes. With these additional modes, new opportunities and challenges in data assimilation are bound to arise.

2.2. Dominant processes

One of the most fascinating aspects of the physical sciences is how different processes come to dominate at different scales, despite the underlying physics necessarily being the same. This is a familiar theme in the study of flows through geological porous media, where considerable research has focused on how pore-scale displacements aggregate into multiphase flow behavior at the field scale. As dominant processes change, so too does the strength and nature of their interactions.

A similar transition can be expected in the transition from the field scale to the regional scale. Since within standard poromechanical models of geological rocks, pressure and mechanical stresses propagate faster than fluid displacement and hence have a large radius of influence, it is to be expected that these are also the processes that first experience significant regional scale interaction. An initial starting point is, therefore, to consider that the regional scale problem, to first order, is a poromechanical system.

On a longer timescale, flow and transport (both of mass and energy) will also start to interact on the regional scale. Such regional scale concerns have already been raised in the context of long-term storage

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(both nuclear waste and CO_2). However, regional scale interactions of flow can also arise on shorter timescales whenever there exist long-range flow networks, such as tunnel structures arising through anthropogenic mining or because of reactive transport in karst formations.

2.3. Upper and lower model boundaries

While the precise distances associated with the regional scale will vary between locations, the examples described in Section 1 all involve processes and interactions on the scale of 50-100 km in horizontal extent. This scale is comparable to the thickness of the crust, and is large enough that the curvature of the Earth's surface starts becoming relevant (about 1 degree).

The vertical extent of a regional scale model must thus be chosen so that the actual dominant processes within the domain are not overshadowed by the somewhat arbitrary restrictions of the vertical extent of the modeling domain. As such, it seems natural that the upper boundary should coincide with the ground surface be it on land, or the seafloor at sea. This choice has the advantage that since the boundary is in contact with either air or water, the boundary conditions can be stated with relatively low uncertainty. On the other hand, this boundary condition immediately brings the attention to the interaction between climate and the subsurface, and particularly the impact of climate change (melting of glaciers, sea-level rise, and changes in precipitation patterns) on regional scale subsurface modeling.

The depth of the lower boundary is less obvious and may well depend on the processes considered and the mechanical stiffness of the geological layers. However, if the lower boundary is relatively shallow, such that the resulting regional scale model has a high aspect ratio, one should expect that the lower boundary conditions must be chosen carefully.

2.4. Model equations

The main equations used to model flow and mechanics in porous media trace their roots back to the 19th century, and were equipped with substantial additional theoretical context through the 20th century. One result of these theoretical and experimental efforts was highlighting the importance of understanding how geometric features at one scale aggregate into constitutive laws at a larger scale. Classical examples when moving from the laboratory to the field scale include the upscaling of non-linear constitutive laws such as relative permeability and capillary pressure, and the emergence of length-scale dependent macro-dispersion as a representation of subscale mixing phenomena.

We thus appreciate that most processes in porous media must *ab initio* be conceptualized as multiscale, from which it may, depending on the concrete processes of interest, be sufficient to reduce the complexity to two-scale or even a single-scale model. Writing the governing equations for basin scale modeling of subsurface systems is no exception. At the largest scale, the balance laws for mass, energy and momentum must certainly be honored, yet whether the constitutive laws can be established at this scale, or must be resolved by resorting to an appropriate multiscale framework where the field scale is explicitly represented, remains an open question, that will likely not have a universal answer.

Some of the particular challenges that arise on the regional scale, which are not present to the same degree at the field scale, is the interaction between geomechanics as a dominant process, and the domain being essentially a slightly curved thin layer (the upper crust) attached to a substrate (the rest of the earth). Thus, we can expect that poroelastic plate theories may play some role, as well as mixed-dimensional mechanical models. At the same time, within this domain, it may be natural to resolve features that themselves have large aspect ratios, such as faults (quasi-2D) or wells and tunnels (quasi-1D).

2.5. Versatile and efficient computational algorithms and physics-data integration

The computational demands of large-scale subsurface modeling are substantial. Numerical simulations must resolve highly non-linear couplings between diverse physical processes across extensive spatial domains and timescales. If aiming for a fully resolved simulation, advanced and massively parallel numerical approaches and high-performance computing architectures are essential to handle the

massive datasets and computational complexity of regional scale subsurface modeling. In addition, models at a regional scale require high-resolution input data that are frequently sparse, uncertain, and difficult to acquire. Consequently, parameter estimation and model validation remain challenging, with uncertainties propagating through predictive simulations. Computational learning techniques have proven capable of deriving models from huge amounts of data. However, data-driven methods require careful consideration, particularly in ensuring the explainability of predictions and adherence to physical laws, such as the conservation of energy.

As an alternative, and keeping the substantial impact of high-performance computing in mind (9), computational saving can be sought by relying on coarser simulation strategies, aiming at either only resolving a coarse level of model equations, or by realizing a multiscale computational algorithm. The feasibility and accuracy of such approaches have yet to be determined.

2.6. Applicability

Reviewing the open issues raised in the preceding sections, one surmises that regional scale subsurface modeling and simulation capability is far from established. Nevertheless, it is meaningful to address what expectations one may have of this emerging field.

As a baseline, all models can be considered as repositories of knowledge, containing data, physical understanding, and/or numerical algorithms. A mature regional scale model will therefore at a minimum be a database of "all relevant knowledge". Despite this minimum capability, this is still of great utility in providing a baseline knowledge of regional scale systems, from which deviations and disruptions can be benchmarked.

Looking past the baseline, models gain power when they become interactive digital representations of the physical system. When this representation has low to moderate accuracy, the applicability lies in history matching and hindcasting, thus aiding the understanding of why and how we have arrived at the present state. As the digital representation gains accuracy, explorations of future scenarios become meaningful, aiding planning and management of our subsurface resources. Thus, the value of regional scale modeling can be clearly established, well before the digital representations become accurate to provide quantitative forecasts of system response.

3. RESEARCH PATHWAYS TOWARDS ESTABLISHING REGIONAL SCALE SIMULATION TOOLS

The preceding two sections of this perspective have pointed to regional scale subsurface modeling as a topic of emerging importance, and one that raises new challenges that need to be addressed and resolved. In this section, we point out concrete research problems that we believe will be useful as points of departure for addressing these challenges.

Identification of a proper modeling paradigm, encompassing dominant processes, domain size, and governing equations, can inherently be addressed from either a top-down or bottom-up perspective. A top-down avenue of research starts with defining the appropriate regional scale geometry and variables, and then constraining the problem based on indisputable physical laws such as conservation laws for mass, energy and momentum. Model closure is then obtained by postulating constitutive relationships based on arguments of symmetry and invariances, dissipative processes and lowest-order approximations. Such top-down approaches have been successfully applied within many branches of porous media research (1). In contrast, a bottom-up avenue of research will take the field-scale models as a starting point and try to directly derive the regional scale equations from these. Whenever such an approach leads to explicit equations on the regional scale, we refer to this as upscaling, and when the regional scale equations are implicitly defined, we refer to this as multiscale modeling. Both upscaling (2) and multiscale modeling (12) have been successfully applied to address issues in porous media, including informing field-scale models based on core-scale processes.

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We do not expect the subsurface at the regional scale to be static, in the sense that a linearized model will be adequate to resolve all processes of interest. Thus, non-linearities will certainly play an important role. Such non-linearities often arise because of coupled processes, such as fault reactivation (coupling to flow and mechanics), changes in the chemical or biological environment (coupling between transport and flow), or large-scale subsidence (changes in the domain geometry and boundary conditions). Whenever these non-linearities lead to degeneracies, such as, e.g., regions of vanishing permeability or mechanical strength, the governing equations change character and may even fail to remain well-posed. Thus, understanding the coupled processes, and their implications for the model, is an important question to resolve. These issues also feed into the design of simulation software, as the methods for resolving (locally or globally) non-linearities and degeneracies in the discrete systems of equations are crucial drivers of computational cost and place constraints on code versatility.

Further advancements in numerical algorithms, uncertainty quantification, and data integration methodologies are critical to improving the predictive capabilities of subsurface models at regional scale. An attractive approach starts by establishing a systematic framework for integrating information from diverse data sources into the modeling-simulation-analysis cycle, while fostering a proactive synergy between physics-based and data-driven computational paradigms. This will allow for a deeper understanding, more accurate predictions and more reliable decisions to be made.

We cannot avoid mentioning the crucial issue of data availability. Given that various subsurface usages may be subject to differing reporting requirements across jurisdictions, the curation and homogenizing of the data presents a highly complex and non-trivial task. Moreover, since much data may be missing—whether related to human activities or geological details—all data must be interpreted within appropriate contexts of uncertainty. Meaningfully handling and accessing such cross-sectorial, cross jurisdictional, and multimodally uncertain data will undoubtedly give rise to research challenges.

Finally, we understand that a full resolution of the issues raised in Section 2 by theoretical and computational advances alone appears unlikely. To some extent, data-based modeling approaches must therefore be integrated so that the relative strengths of physics-based mechanistic models and statistical analysis of available data and observations can be utilized to their full potential. Such hybrid analysis and modeling frameworks are currently being developed across science and technology, yet specialized adaptations to the particularities in data and equation structures that arise in regional scale subsurface modeling will undoubtedly be necessary.

4. CONCLUSIONS

Our perspective is that the research community must rise to the occasion, and take a proactive approach to regional scale subsurface modeling. We envision a modeling scale that closes the gap between field-scale simulation and lithospheric modeling, with a regional scale covering 100s of km in the horizontal direction, and up to 10km in the vertical direction. To realize this vision, challenges must be overcome in terms of data, modeling and simulation tools.

Advancement of knowledge and regional modeling capabilities, supported by a knowledgeable community, will enable the safe, efficient and equitable exploitation of subsurface resources required for the furtherment of modern society.

STATEMENTS AND DECLARATIONS

Author Contributions

All authors contributed to the conceptualization and writing (review and editing). IB and JMN wrote the original draft and were responsible for funding acquisition.

Conflicts of Interest

There are no conflicts of interest to declare.

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