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A review of applications of fractional calculus in Earth system dynamics

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ABSTRACT

Fractional calculus has been used to model various hydrologic processes for 15 years. Yet, there are still major gaps between real-world hydrologic dynamics and fractional-order partial differential equations (fPDEs). In addition, the applicability of fPDEs in the broad field of Earth dynamics remains obscure. This study first reviews previous applications and then identifies new research directions for fPDEs simulating non-Fickian transport in both surface and subsurface hydrology. We then explore the applicability of fractional calculus in various anomalous dynamics with a wide range of spatiotemporal scales observed in the solid Earth, including internal dynamics (such as inner core rotation, outer core flow, mantle convection, and crustal deformation), large-scale surface dynamics (in fluvial, Aeolian, and glacial systems), and small vertical-scale surface kinetics (in crystal growth, rock/mineral weathering, and pedogenesis), where driven forces, previous modeling approaches, and the details of anomalous dynamics are analyzed. Results show that the solid Earth can provide an ideal and diverse base for the application of fractional calculus and fPDEs. Complex dynamics within and across spatiotemporal scales, multi-scale intrinsic heterogeneity, and intertwined controlling factors for dynamic processes in the solid Earth can motivate the application of fPDEs. Challenges for the future application of fPDEs in Earth systems are also discussed, including poor parameter predictability, the lack of mathematical specification of bounded fractional diffusion, lack of intermediate-scale geologic information in parsimonious and upscaling models, and a lack of models for multi-phase and coupled processes. Substantial extension of fPDE models is needed for the development of next-generation, solid Earth dynamic models, where potential solutions are discussed based on our experience gained in the development and application of fractional calculus and fPDEs over the last decade. Therefore, the current bottleneck in the application of fractional calculus in hydrologic sciences should not be the end of a promising stochastic approach, but could be the early stage of a decade-long effort filled with multiple new research and application directions in geology. This conclusion may shed light on the bottleneck challenging stochastic hydrogeology, where the advanced stochastic models (with more than 3500 journal publications in the last three decades) have not significantly impacted the practice of groundwater flow and transport modeling.

1. Introduction

Fractional calculus and corresponding fractional partial differential equations (fPDEs) have drawn increasing attention in various scientific disciplines involving heavy-tailed dynamics for two decades [1–3]. When the integer-order derivative in a standard mass, momentum or energy conservation model is replaced by a fractional-order derivative, the local variation of mass, momentum or energy (which usually cannot be measured exclusively) can be upscaled, resulting in a nonlocal fPDE with spatially or temporally averaged parameters that can efficiently capture the heavy tailed dynamics without the prohibitive burden of mapping detailed system heterogeneity. After 20 years of application in the natural sciences and tremendous efforts in the development of theories, models, and solvers for fPDEs (e.g., google scholar showed 216,000 publications in December 2016 containing "fractional partial differential equations" AND "application"), we now need to review these applications to better understand the nature of anomalous dynamics and improve previous models and to identify future research directions for fractional calculus and fPDEs. Specifically, what are

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the future application areas of fPDEs, and what type of models and mathematical theory are needed in the next decade? This study attempts to address these challenges from a geological perspective, which is perhaps the most complex and broad discipline in the natural sciences.

Geology is focused on planet Earth. The Earth system is a dynamic, global interconnecting web of physical, chemical, and biological phenomena involving the solid Earth, the hydrosphere, and atmosphere, which transform or modify unidirectionally or periodically at various time scales (varying from seconds to billion years) and spatial scales (from atom level to continental scale). Fractional-calculus-based models have been successfully applied to capture various real-world anomalous processes in the hydrosphere (see, for example, the review by Zhang et al. [4]). Anomalous transport has been observed for tracers moving alongside water in natural geological media, including soil, rivers, and aquifers (see references and brief review in Section 2). Such anomalous behavior may persist or evolve when the transport of dissolved pollutants spans a wide range of spatiotemporal scales, where drivers of anomalous dynamics (such as hydraulic properties) exhibit intrinsic multi-scale heterogeneity.

This study focuses on both the hydrosphere and the solid Earth. Applications of fPDEs help to understand the nature of liquid phase contaminant transport in the hydrosphere, one of the fundamental and challenging tasks in hydrology. Further development and applications of fPDEs to modeling other complex hydrologic processes are needed, which will be discussed in this study. We then explore the potential extension of fractional calculus in solid Earth applications, another major component of the Earth system that has received little attention so far in the application of fPDEs. The solid Earth contains intrinsic multi-scale physical, chemical, and/or biological heterogeneity, which may provide an ideal and diverse base for developing and testing the application of fPDEs and nonlocal transport theories.

The rest of this work is organized as follows. In Section 2, we briefly review the hydrologic processes that can be characterized by fPDEs and explore the underlying physical reason for favoring the application of fPDEs. Future applications of fPDEs in both surface and subsurface hydrology are then discussed. In Section 3, we explore a broad range of anomalous geological dynamics (with fast displacement, elongated delay, or a mixture) in the solid Earth, by focusing on their underlying driving forces and mechanisms, which can guide the development of physical-based models using fractional calculus. Both Earth's internal dynamics and Earth surface processes are discussed. In Section 4, we discuss the intrinsic challenges and potential solutions for the application of fPDEs in quantifying various dynamics in the solid Earth and hydrosphere identified in the previous sections. Conclusions are finally drawn in Section 5. We believe that this study can provide broad research and application areas in the geological sciences for fractional calculus throughout the next decade.

2. Application of fPDEs in hydrosphere

2.1. A brief review: spatiotemporal nonlocal signal in water flow and solute transport

Fractional calculus, which is as old as its integer-order counterpart, replaces integer numbers with real numbers in differential and integration operators [5,6]. The fractional-derivative operator was used to generalize Fick's law to capture super-diffusion by the physics community, and has remained an active research area for simulating anomalous diffusion [1,2]. There are two types of fractional-derivative models in hydrology. The space fractional-derivative model captures the fast movement (or super-diffusion) of targets (such as tracers), while the time fractional-derivative model captures delayed motion due likely to retention, compared to its integer-order counterpart. The fPDEs are attractive in simulating hydrologic processes since they are nonlocal, upscaling models that can efficiently capture sub-grid heterogeneity and the spatial correlation of heterogeneity [4].

We first explore knowledge obtained from previous applications of modeling flow and transport in the hydrosphere with fPDEs, in the liquid component in the Earth system. Since the pioneering work of Benson [7], Meerschaert et al. [8], and Benson et al. [9], who introduced the fractional-order diffusion model for super-diffusive solute transport in hydrology (see also Meerschaert et al. [10]), fractional-derivative models had been developed, approximated, and applied to quantify many procedures in water cycles. We group these procedures into three regimes: subsurface (i.e., porous media and fractured rock masses), soil, and surface, and we review each of them in the following paragraphs.

Subsurface flow and transport modeling has benefited from the application of fPDEs, considering the inefficiency of standard Fickian-based transport models in capturing well-documented non-Fickian transport in natural aquifers. Two representative aquifers have been explored extensively: alluvial aquifer/aquitard settings and fractured aquifers. In a typical alluvial deposit, spatially interconnected ancient channels (which can extend up to hundreds of meters for straight-type channels) provide preferential flow paths and motivate super-diffusive contaminant transport [11], which are efficiently characterized by space fractional advection-dispersion equations (fADE) [12]. Meanwhile, surrounding low-permeability floodplain deposits retard pollutant transport and cause significant sequestration or sub-diffusion, which can be modeled by the time fADE [13–15]. In erratic, multi-dimensional fractured media constituting 90% of natural aquifers, fast motion in fractures and multi-rate mass exchange due to matrix diffusion can result in a mix of super- and sub-diffusion, which can be modeled by spatiotemporal fPDEs [16,17]. The fPDEs are especially attractive when describing complex transport behavior in fractured media at regional scales, without introducing the computational burden of explicitly incorporating individual rock fractures [18].

Natural soil exhibits complex internal structures and heterogeneous hydraulic properties, such as unsaturated hydraulic conductivity, which can vary by orders of magnitude in a short distance. Macropores consisting of earthworm burrows, root channels, interconnected cracks, interaggregate pores, and/or other local high-permeability zones in aggregated field soils (which are typically shorter than $\sim$10 m in natural soil along a hillslope) can provide non-equilibrium preferential pathways for water and chemicals. Meanwhile, micropores, clay minerals, and/or other soil matrix regions tend to adsorb solute particles and challenge local equilibrium assumptions that support standard flow models. The existence of macropores and/or micropores can result in non-Boltzmann scaling of water flow through horizontal soil columns, which cannot be efficiently captured by the Richards equation (assuming normal diffusion). A fractal Richards equation, which is similar to the fPDE, was proposed by Sun et al. [19] to quantify both super- and sub-diffusive, non-Boltzmann scaling in unsaturated soil. The fractal nature of soil also motivated Pachepsky et al. [20] to propose a time-fractional Richards equation without distinguishing the mobile and immobile status. The fractional Green-Ampt model was also proposed by Voller [21] to account for the non-monotonic rate of infiltration through natural soils.

Surface hydrologic processes, including surface runoff and sediment transport in rivers, exhibit complex patterns due to spatiotemporal memories and have been recently modeled by fPDEs. For example, Harman et al. [22] developed a subordinated kinematic wave equation (KWE) to model heavy-tailed flow responses (with a power-law memory function) from heterogeneous hillslopes. Zhang et al. [23] proposed a spatiotemporal fractional-order

Table 1
Hydrosphere: hydrologic processes in subsurface aquifers, soil, and land surface.

Group	Representive process	Major triggers/dominant factors	fPDEs developed before	Future extension
Subsurface	(1) Conservative contaminant transport (2) Bimolecular reaction	(1) Mobile zone due to interconnected high-permeable deposits (2) Immobile zone due to clay/matrix (3) Incomplete mixing of reactants	Standard fPDEs	(1) Transient flow (fractional-order flow equation) (2) FPDE for complex chemical reactions (fractional-order reactive model) (3) Variable density flow
Soil	Moisture movement with non-Boltzmann scaling	(1) Macropores for fast movement of water and chemicals (2) Micropores or soil matrix for retention	(1) Fractal or fractional Richards equation (2) Fractional Green-Ampt model	(1) Soil aeration (Fractional-order gas diffusion model) (2) Heat conduction (Fractional-order Fourier law) (3) Multi-phase transport (Fractional-order Raoult's law)
Surface	(1) Surface runoff (2) Bedload sediment transport in rivers	(1) Random distribution of soil hydraulic properties, topography, land cover, etc. (2) Turbulence and river bed properties	(1) Fractional-order continuity model (2) Fractional-model for sediment transport	Biological and ecological process in rivers

continuity equation to quantify scale-dependent overland flow, by adding power-law memory kernels to the standard KWE. Many efforts have been made to develop and apply the fPDEs to efficiently quantify the random motion and burial periods of bedload sediments along natural river beds, by extending previous models for bedload transport (for an incomplete list, see Bradley et al. [24] and Zhang et al. [25] for field applications). Other nonlocal models, such as the Exner-based Master Equation [26] and the elastic Langevin equation [27], were also proposed for bedload transport. The above processes are summarized in Table 1.

The above applications show that the fPDEs applicable for hydrosphere dynamics exhibit similar forms. For example, the one-dimensional, spatiotemporal fPDE model that can distinguish the mobile and immobile status of (water, chemical, or sediment) particles takes the form [28]:

$$\frac{\partial P_m}{\partial t} + \beta \frac{\partial^{\gamma,\lambda_T} P_m}{\partial t^{\gamma,\lambda_T}} = -v\frac{\partial P_m}{\partial x} + D\frac{\partial^{\alpha} P_m}{\partial x^{\alpha}}, \tag{1a}$$

$$\frac{\partial P_{im}}{\partial t} = \frac{\partial^{\gamma,\lambda_T} P_m}{\partial t^{\gamma,\lambda_T}}, \tag{1b}$$

where P $[ML^{-3}]$ is the density (or chemical concentration for pollutant transport process); the suffix "m" (or "im") denotes pollutant in the mobile (or immobile) phase; β $[T^{\gamma-1}]$ is the total capacity coefficient; $0<\gamma<1$ [dimensionless] is the order of the time fractional derivative; λ_T $[T^{-1}]$ denotes the truncation parameter in time; v $[LT^{-1}]$ is the average velocity; D $[L^2T^{-1}]$ is the effective diffusion coefficient; and $1<\alpha<2$ [dimensionless] is the order of the space fractional derivative. When $\gamma=1$ and $\alpha=2$, model (1) reduces to the standard advection-dispersion equation (ADE) with linear equilibrium sorption during transport (and a unit distribution coefficient). Model (1) (most times with $\lambda_T=0$; i.e., without tempering in the stable density) was used to simulate pollutant transport in aquifers [9,4,14,29], pollutant transport in fractured media [16,18], rainfall properties [30], and water wave propagation and flow in pipes [31,32]. Model (1) and its extension were also used to simulate sediment transport in rivers [24,25,33] and surface runoff along heterogeneous hillslopes [23]. In the following we will discuss the potential extension of model (1) for simulating other dynamics in the Earth system. We note that a mechanistic physical model is preferred to describe Earth system dynamics, and fractional calculus can be added into the model by either developing a nonlocal physical model, or adding memory impact to the original, local model. In the first approach, the spatial and/or temporal convolution of the research target with nonlocal kernels may lead to specific fractional-derivative models (see further discussion in the next section). In the second approach, the subordination approach (an efficient mathematical tool for transferring the system from physical time to a new operational time [34,35]) can be used to add temporal and/or spatial memory to the traditional PDE governing the Earth system dynamics of interest. It is also noteworthy that model (1) with only time nonlocality (i.e., $\alpha=2$) is a subset of the general time-nonlocal conservation model. Particularly, model (1) with $\alpha=2$ reduces to the multi-rate mass transfer (MRMT) model with upper-truncated mass transfer rates [36], the hydrologic-version of the continuous time random walk (CTRW) with an exponentially-truncated memory function [37], and a specific case of the phase exchange model [38]. Model (1) with only space nonlocality (i.e., $\gamma=1$) is a subset of the convolution-Fickian transport model [39]. Hence, the potential extension of the fPDE discussed in this study may also shed light on other nonlocal models. We note that the full version of model (1) separates sub- and super-diffusion driven by different mechanisms, and as will be shown below, it can be extended to nonstationary systems.

In summary, hydrologic processes occurring in the subsurface, soil, and surface can exhibit non-Fickian behaviors, mainly due to multi-scale heterogeneity embedded in hydrologic and hydrogeological properties. Note that the hydrologic processes discussed here include not only solute transport (where the non-Fickian behavior is likely due to nonlocal, mechanical dispersion and/or solute retention), but also water movement (where the non-Darcy behavior is likely due to differential advection and/or water retention). For example, Silva et al. [40] showed that dual-domain flow processes can give rise to nonlocal models (see their Eqs. (5) and (6), which are similar for both water flow and solute transport with multiple mass-transfer rates) and capture non-equilibrium flow/transport behavior. Although the exact driving forces and transport mechanisms for these non-Fickian dynamics differ apparently from subsurface aquifers to surface rivers (see Table 1), these hydrologic processes can be conceptualized as stochastic processes with random displacement between random waiting periods, leading to the same mathematic description underlying the fractional-derivative based stochastic model. It is also noteworthy that the fPDE models can differ subtly from subsurface to surface processes, likely due to the discrepancies of scale and flow velocity in different regions. For example, water in aquifers can move as slowly as $10^{-3}\sim10^{0}$m/day, and the preferential pathway may be longer than the plume size (hundreds of meters) in most monitoring periods (typically shorter than a few years) due to lateral continuity, requiring the fPDE model with a standard stable density. Preferential pathway in soils or rivers (typically in the range of $10^{-1}\sim10^{1}$ m), however, can be much shorter, and hence tempered stable density should be applied in the fPDE to describe solute movement with finite jumps, as discussed in Meerschaert et al. [41].

2.2. Potential future research and application directions of fPDEs in hydrosphere

The application of fractional models in the hydrosphere is reaching a bottleneck, similar to the other stochastic hydrogeology approaches that have been developed and applied for 40 years (including perturbation methods, moment equation approaches, Monte Carlo methods, and PDF-based methods [42]), likely due to a lack of incorporation of local hydrogeologic properties, limited information on the geologic architecture, and/or lack of data assimilation, including measurements of dependent variables [43] (see further discussion in Section 4). In other words, an information-rich and hydrogeology/practice-oriented fPDE model might be the future research direction for fractional calculus in the hydrosphere. How to incorporate geologic information into the fPDE models will be discussed further in Section 4.2. Here we explore the major research areas in the hydrosphere that have not yet been a focus of the fractional approach.

Further research and application of fPDEs are needed to describe real-world reactive transport, multi-phase transport, variable density flow, energy transfer, and coupled flow and transport in the hydrosphere. For example, previous applications of fPDEs in hydrologic dynamics are limited to conservative tracers and liquid-solid phases. Fractional calculus-based diffusion theories have not been applied for real-world reactive dynamics beyond fundamental, second-order bimolecular reactions [44-46]. The challenge is that chemical reactions occur at the molecular level, which cannot be reliably upscaled in a stochastic model focusing on larger-scale plume spreading. One possible solution might be the Lagrangian approach for mixing-controlled reaction kinetics [47] combined with updated transport models [48], which lead to a multi-scale fPDE model. Another way to build a multi-scaling model is to combine the fractional model (for large-scale transport) and mixing-limited (mixing-ratio based) reactions for multispecies [49,50] or the lamellar description for mixing [51]. In addition, multiple-phase transport for volatile chemicals (i.e., pesticides) in natural soil remains a historical challenge in numerical modeling, which may require a fractional-version of Raoult's law or other improved formulas for gas-water phase partitioning (that can characterize the possible multiple rate partition). Soil aeration may also require a fractional-version of a gas diffusion model, considering (1) the significant discrepancy of gas diffusion capability between void space and water films in the vadose zone, and (2) the obscure internal structure and connectivity of natural soil that cannot be reliably measured. In addition, fPDEs may also be needed to capture heat conduction in unsaturated soils, where the standard Fourier's law can be generalized by a fractional-order conductive heat flux to account for non-uniform conduction. Similar generalizations have already been proposed by several researchers for the Stefan model of latent-heat transfer [52-54]. The challenge of soil systems is that unsaturated soil can be much more complex, since it contains multiple phases and scales of heterogeneity. When water turns partially into ice in winter, the heat flux is altered significantly, challenging previous heat conductive models. In addition, how to develop fPDEs to capture variable density flow, and how to couple transient flow and transport processes (which may require the coupled fractional flow equation and fADE for non-steady and nonuniform flow), remain unknown. These processes can lead to future research topics of fractional calculus.

In addition, complex dynamics can also be observed in other aquatic processes. For example, in biogeochemical sciences, the reliable quantification of transport and transformation of dissolved organic matter (DOM) in rivers/streams remains a historical challenge, even at the reach scale, due to complex biological (i.e., microbial consumption) and chemical (such as photosynthesis) reactions whose rates, sources, and types cannot be measured extensively or even fully understood at present. Similar challenges exist for quantifying aquatic dynamics in molecular and isotopic geochemistry, and regional, environmental and exploration geochemistry. High uncertainty and limited information in aquatic geochemical processes requires efficient stochastic models, motivating the future application of fPDEs. The knowledge gained in subsurface contaminant transport modeling over the past decade may guide the development of fPDEs for the above chemical kinetics. The necessity of fractional calculus in geology may be much stronger than expected, with the last decade being only the beginning of the application of fPDEs, even for the well-studied hydrosphere.

A generalized nonlocal model might be needed to account for various memories in anomalous dynamics. This might be done by generalizing the standard fPDE (1) after combining the multi-rate mass transfer model with a general memory function [55,36] and with the nonlocal dispersive constitutive theory with a general kernel in space [56,39,12]:

$$\frac{\partial P_m(x,t)}{\partial t} + \beta \frac{\partial P_m(x,t)}{\partial t} * f(t) = -\frac{\partial}{\partial x}[\nu(x,t)P_m(x,t)] + \frac{\partial}{\partial x}\int_0^t \int_R g(y,t,\tau)\frac{\partial P_m(x-y,t-\tau)}{\partial (x-y)}dyd\tau, \tag{2a}$$

$$P_{im}(x,t) = \int_0^t f(t-s)P_m(x,s)ds, \tag{2b}$$

where the symbol $*$ denotes convolution, $f(t)$ $[T^{-\gamma}]$ is the memory function defining the distribution of rate coefficient for mass exchange between the mobile and immobile zones, g is the memory kernel for diffusive jumps in space, and R $[L]$ denotes one-dimensional Euclidean space. When the velocity remains constant and the two memory functions take the following specific forms:

$$f(t) = \int_0^t e^{-\lambda_T r}\ \frac{\gamma\ r^{-\gamma-1}}{\Gamma(1-\gamma)}\ dr, \tag{3a}$$

$$g(y,\tau) = \frac{D\ \delta(\tau)\ H(y)}{\Gamma(2-\alpha)\ y^{\alpha-1}}, \tag{3b}$$

the generalized nonlocal model (2) reduces to the fPDE model (1). In the kernel (3b) for dispersive flux in space, the Heaviside step function $H(y)$ defines upstream space nonlocal transport (if large backward diffusion is negligible), and the Dirac delta function $\delta(\tau)$ defines a time-local kernel. Model (2) provides the flexibility to select appropriate kernels to describe various memory functions in time and space that can lead to the complex dynamics observed in natural geological media, including those discussed below.

3. Solid Earth dynamics: processes and potential applicability of fractional calculus

We separate the solid Earth processes into three groups, based on their location and scale. Internal Earth dynamics cover motion from the inner core to the crust (Table 2). Large-scale Earth surface dynamics occur at the land surface (Table 3). Lastly, some solid Earth processes have limited vertical scales, such as the chemical weathering of rocks and minerals.

3.1. Earth internal dynamics

3.1.1. Inner core rotation

Earth's solid, anisotropic inner core, consisting of iron alloy with a radius of about 1220 km, resides concentrically within the much

Table 2
Earth internal dynamics.

Internal dynamics	Major driving force	Spatiotemporal scales	Major triggers	Previous models	Anomalous dynamics	Possible fPDE
Inner core rotation	Magnetic coupling between the electrically conductive inner core and the geomagnetic field	10^3∼10^6 m 10^0∼10^4 year	Coupled with other processes, such as outer core dynamics	(1) Deterministic, reverse model for rotation rate (2) Part of the geodynamo models	Not clear due to limited data	(1) A fractional-order angular momentum model (2) Fractional-order dynamo models
Outer core	(1) Energy provided by the slow growth of the inner core (2) Heat flow from the inner core	10^3∼10^6 m 10^0∼10^4 year	- Convection due to heat flow from the inner core - Rotation is supplied by the Coriolis effect	Numerical geodynamo model	Non-Gaussian distribution of the axial dipole	(1) A fractional dynamo model (2) A continuous time random maximum model
Lower-mantle flow	Buoyancy	10^4 ∼ 10^7 m 10^6 ∼ 10^9 year	Slab push; plate pull	Multi-dimensional mantle flow model	Anomalous transport caused by multi-scale cycles of mantle flow	fPDE is needed to release the prohibitive computational burden of current models
Upper-mantle flow	Buoyancy	10^4 ∼ 10^6 m 10^5 ∼ 10^7 year	(1) Large-sale movement of plates; (2) Small-scale convection may dominate upper-mantle deformation	(1) Two-component flow models (2) Various software suites for 1-d to 3-d mantle flow modeling, i.e., CitComs which is the standard thermal-chemical convection model [Tan et al., 2014]	Thermal or chemical convection can exhibit anomalous behavior in heterogeneous systems	Fractional version of the thermal-chemical convection model
Crustal deformation	Stress (compression, tension, and shear stress)	10^1 ∼ 10^4 m 10^{-1} ∼ 10^2 year	Temperature, pressure, deformation rate, and rock composition	Elasticity equation	Rock deformation affected by internal and external factors, hard to be predicted by deterministic models	(1) Fractional elasticity equation (2) Spatiotemporal fPDE model may capture mountain uplift

Table 3
Earth surface dynamics: properties and potential application with fPDEs. In the column labeled "Spatiotemporal scale", the units are meters for space and years for time.

Earth surface dynamics	Major driven force	Spatiotemporal scales	Major triggers	Current model	Anomalous dynamics	Possible fPDE
Mass wasting	Gravity	10^{-1}∼10^3 m 10^{-7}∼10^2 year	Excessive water, and earthquakes	Local momentum equation	Competing anomalous transport with fast moving and long retention stages	Two-phase coupled fPDE model
Aeolian sand dune growth and migration	Wind	10^0∼10^4 m 10^{-4}∼10^2 year	Turbulent wind flow, sand supply, and sand interaction	Standard transport model under variable wind velocity	Super-diffusion in windward side, and sub-diffusion in leeward side	Turbulent wind + multi-dimensional spatiotemporal fPDE with a space-dependent index
Glacial erosion-deposition	Gravity	10^1 ∼ 10^6 m 10^1 ∼ 10^6 year	Climate, hydrologic condition (i.e., debris concentration and flux) and properties of the underlying bedrock	(1) Standard (the simple power-law) erosion law, valid only for small scale erosion (2) Depositional processes are difficult to model	Potential anomalous transport sensitive to the erosional or depositional process	(1) Fractional-calculus based novel erosion law to capture larger-scale landscape models by upscaling small-scale processes (2) Extend the fPDE for glacial deposits

larger fluid outer core, and rotates 0.2° to 0.3° per year faster than the mantle [57]. Travel-times between seismic body waves show that this rate corresponds to a speed of a few tens of kilometers per year for the inner core around the equator [58]. The slow differential inner core motion (with the rotation rate likely changing on a decadal time scale [59,60]) was long believed to be driven by magnetic coupling between the electrically conductive inner core and the geomagnetic field [60,61–64]. The toroidal field generated by the outer core [61] and convection driven by the temperature contrast between the rigid boundaries of the inner core and/or buoyancy flux may affect the angular velocity and/or growth rate of the inner core [65].

Deterministic models were developed for inner core differential rotation [58,66,67], which are not physical process-based models for inner core dynamics, but inverse models (given seismic wave travel-times) to calculate, for example, the inner core rotation rate and velocity perturbation (see Eq. (2) in Song [67]). The inner core velocity perturbation is a (local) function of many controlling factors, including latitude, longitude, spin axis, time, and depth. In addition, dynamo models were also used widely to calculate angular velocity for inner core coupled with outer core dynamics [60], and are discussed further below.

It is possible to describe the randomness and anisotropy of inner core rotation due to the system heterogeneity using a stochastic model like the vector fPDE, since the impact of system inhomogeneity on target dynamics usually cannot be captured efficiently by standard deterministic models. In addition, solid iron alloy in the inner core can precipitate from the liquid outer core, and such recharge across the outer-inner core interface is not constant but rather changes with time and position, resulting in a random process that challenges the application of deterministic models. A fractional-order angular momentum model might be applied to characterize inner core rotation. The challenge is, however, the limited data in model development and parameterization. Inner core rotation is also closely linked to other large-scale dynamics, especially outer core flow, and therefore, a coupled fPDE model might be needed to simulate the motion of the inner and outer cores.

3.1.2. Outer core flow

The outer core consists of a liquid iron alloy that can flow. According to the geodynamo theory, convective currents in the outer core are driven by heat flow from the inner core and these currents are organized into rolls by the Coriolis force, ultimately generating the Earth's magnetic field [68]. It has also been suggested that the slow growth of the inner core, mentioned in Section 3.1.1, may provide an energy source that helps drive the geodynamo [63]. The outer core dynamics may also lead to geomagnetic reversals, where the temporal interval between subsequent magnetic reverse records is not uniform, but rather random. Multiple components might be contributing to the historic reversal of the magnetic field, where some components are periodic and others are not, resulting in irregular inter-arrival times that might not be reliably quantified by deterministic models.

Outer core convection models were developed to solve coupled equations describing convective motions and dynamo action. For example, in the popular numerical dynamo model "MaglC3" [69], the Navier–Stokes equation in the Boussinesq approximation (for magnetic velocity) takes the standard form, and the convection-transport equation (for both magnetic induction and super-adiabatic temperature) also assumes normal diffusion. Numerical results revealed both Gaussian and non-Gaussian (with apparent tailing behaviors) distribution for the axial dipole, which can cause geomagnetic field reversal. Self-consistent dynamo models were also applied to reproduce geomagnetic reversals [70].

A prospect of fractional calculus for outer core dynamics is to generalize local diffusive terms in the previously developed dynamo models (such as the standard diffusion equations mentioned above) using nonlocal, fractional calculus to efficiently capture the impact of local heterogeneity on outer core convective motions. Considering the extremely limited observation, solutions from previous dynamo models with fine-resolution parameters can be used to guide the development of the fractional-version model. The challenge is that standard dynamo models are extremely difficult to solve. However, when a fractional-order derivative replaces an integer-order one in the governing equations, time and/or space dependent parameters can be upscaled, resulting in constant parameters. This mathematical simplification is similar to the kinematic simplification of the nonlinear dynamo models, and hence, the introduction of fractional calculus may partially relieve the computational burden of the dynamo models.

Another simplification of the self-consistent dynamo models could be the adoption of the continuous time random maximum (CTRM) model, proposed by Benson et al. [71], to quantify the magnetic reverse events. In the CTRM model, the irregular inter-arrival times between magnetic reversals may follow the tempered stable density applied by Meerschaert et al. [41] for hydrologic dynamics, which generalizes the widely used, standard stable density (see, for example, Benson et al. [71]). This tempered stable density is the universal model for travel-time distributions in many hydrological and environmental processes [72,73].

3.1.3. Lower mantle convection

The lower mantle (from a depth of ~650 km down to 2900 km) composition is not precisely known, as samples of inclusions in diamond, which provide our only direct constraints, are sparse [74]. Minerals in the lower mantle are most likely high-pressure equivalents of peridotite and include Fe-periclase, MgSi-perovskite, and CaSi-perovskite (e.g., Kaminsky [75]). Most of the lower mantle is solid, with only a few percent melt, which is likely concentrated in the lower-upper mantle transition zone [76]. Lower mantle convection is slow, likely accommodated by diffusion (non-Newtonian) creep of the Earth's solid silicate mantle, caused by convection currents carrying heat from the interior of the Earth to its surface [77,78]. Different convective models exist. For example, some studies advocated that convection in the mantle is two-layered, with the upper mantle being distinct from the lower mantle [79]. Other studies also suggested whole-mantle convection and/or some type of hybrid model where flow between the upper-lower mantle occasionally "breaks through" [80].

The driving force of mantle flow is the buoyancy force generated by thermally-induced density anomalies [81]. Typical mantle convection speed is <20 mm/year, but it can vary significantly. Deeper mantle convection cycles can be close to 200 million years, while a single shallow convection cycle can be as fast as 50 million years. The convection of lower mantle near the outer core is much slower than the small-scale convection in the upper mantle, likely due to the change of viscosity and pressure with depth.

Numerical models have been developed to simulate mantle flow at regional and global scales. For example, Hu and Liu [82] and Liu and Hasterok [83] applied a four-dimensional (spatial coordinates plus time) model to simulate mantle flow beneath the Americas using a data assimilation approach that incorporates seismic tomography. The grid-based numerical model contains $10^1 \sim 10^2$ million grids and 10^2–10^3 million unknown parameters, requiring challenging computation. Mantle flow may contain multi-scale cycles, which can be a mixture of local, intermediate, and regional cycles. There are also significant spatial variabilities in the lower mantle convection as well. For example, there are regions associated with both "small-scale" upwellings (i.e., plumes) and very massive upwellings (i.e., super-plumes). The spatiotemporally multi-scale mantle convection is similar to the mixed flow lines in groundwater, motivating the application of a nonlocal dynamic model, such as a fPDE.

3.1.4. Upper mantle convection

Upper mantle (from a depth of ~410 km down to the lower mantle) composition and mineralogy are better constrained than that of the lower mantle because xenoliths from volcanic eruptions are available, which can guide the development of numerical models. The upper mantle composition is dominantly peridotite with abundant olivine, garnet, and pyroxene in the upper part and wadsleyite and ringwoodite near the transition into the lower mantle [84]. The mineralogy differences from the lower mantle are mostly due to the lattice structure dependence on temperature and pressure, and to a lesser extent, on slight differences in composition. The upper mantle (including the transition zone) is likely dominated by deformation accommodated by both diffusion and dislocation creep [77,78]. Mineral lattice types affect mineral deformation and flow, which in turn, affect mantle flow dynamics, requiring different physical models between the lower and upper mantle. There is distinction between upper and lower mantle anisotropy, in relation to mineral deformation and flow. Anisotropy might be much more developed in the upper mantle, due likely to the lattice preferred orientation of olivine (dislocation creep), while the lower mantle is mostly isotropic.

Various models have been proposed to simulate upper mantle convection. For example, Frank [85] proposed a two-component convection model to quantify upper mantle movement, with one component representing percolating melt fluid and the other representing a solid plastic flow. Froidevaux and Schubert [86] proposed a one-dimensional $(1-d)$ shear flow model to quantify upper mantle dynamics beneath a continent, by accounting for viscous dissipation as well as a temperature- and pressure-dependent nonlinear mantle rheology. Humphreys and Hager [87] developed a kinematic model to access upper mantle deformation beneath southern California. One of the most commonly used models is the CitComs software suite, originated developed by Moresi and Solomatov [88] and extended by others (see Tan et al. [89]), which can solve thermal-chemical convection governed by the conservation of mass, momentum and energy (i.e., standard partial differential equations or PDEs). Similar software suites, including source packages and user manuals, such as ASPECT, ConMan, Ellipsis3D, and HC developed to model mantle dynamics, can be obtained from the Computational Infrastructure for Geodynamics (https://geodynamics.org/cig/software/). Considering the inefficiency of standard conservation models in capturing the nuances of thermal-chemical convection in a regional-scale heterogeneous system, fPDEs can be a potential alternative for upper mantle convection modeling.

In addition, the dominant driving force associated with upper mantle convection is debated. While it has long been believed that the strongest deformation in the mantle was controlled by large-scale plate motion (i.e., the push of mid-ocean ridges, or slab pull), recent high-resolution seismic imaging has revealed that upper mantle flow beneath the ocean's tectonic plates may be dominated by small-scale convection [90]. Hence, both large- and small-scale dynamics need to be accounted for when modeling upper mantle convection, challenging the traditional modeling approach and motivating the application of stochastic models such as the fPDE efficient for multi-scale dynamics.

3.1.5. Crustal deformation

The continental crust is highly heterogeneous, but on average, is granodiorite in composition [91]. Crustal deformation produces geologic structures such as joints, faults, folds, and foliation. Both brittle deformation (i.e., cracking and fracturing) and ductile deformation (i.e., bending and flowing) occur in rocks subjected to stress. The type of deformation is mostly controlled by the strain rate, temperature, and pressure with lesser dependence on mineralogy. Brittle deformation is dominant in the upper crust, and ductile deformation is dominant in the lower crust, due to the depth-dependent temperature and pressure. Oceanic crust also undergoes all the same deformation processes as continental crust (i.e., fracturing, flowing, etc.).

Crustal displacement can be calculated by the elasticity equation, which was developed into the popular software PyLith [92]. Other models and software suites for short-term crustal dynamics can be obtained from the Computational Infrastructure for Geodynamics (https://geodynamics.org/cig/software/). It is noteworthy that the elasticity equation was built upon the standard conservation of momentum, which may not be efficient if anomalous deformation dominates. In addition, brittle fracture development can also be affected by other factors, such as the motion of thermal fluids, rock mechanics, and regional press fields (tectonics). Therefore, deterministic prediction of fracture formation and extension is difficult even at the sedimentary scale. The hydrofracing technique, used to enhance oil/natural gas productivity, is another example of where this type of assessment is important. Stochastic models should be used to account for the random deformation (transient or long-term) of rocks under real-world conditions.

Crustal deformation can lead to mountain uplift related to subduction, continental collision, and continental rifting. The mantle cannot maintain high shear stresses; therefore, the crust beneath mountains approaches isostatic equilibrium over long time frames. Thus, crustal thickness and density variations are critical parameters for modeling mountain building. Such modeling is complex due to the involvement of heterogeneous deformation mechanisms, transient behavior, and feedback mechanisms (e.g., Beaumont et al. [93]). For example, during the long-time scale of a collisional orogeny or convergent-margin orogeny, horizontal compression causes the crust to thicken vertically, which in turn, affects the geothermal gradient. Removal of lithospheric mantle from the base of a plate can also cause the remaining lithosphere to rise and form mountains due to the replacement of dense cold rock with less dense hotter rock. Shorter time scale processes can also cause surface uplift or mountain building. For example, the addition of igneous rock to the crust (i.e., volcanic eruption or magmatic intrusion) can generate mountains resulting from the addition of high temperature, low density rocks. In rift environments, hot asthenosphere rises and heats the lithosphere, resulting in uplift. Thermal expansion in the crust due to collision, rifting, and rupture is typically a short-term mechanism for mountain uplift. It is our own expectation that the rate of mountain uplift can dramatically change with time, with fast periods being intermingled with relatively stationary periods or even erosional events. Hence, mountain uplift might be better described by a spatiotemporal fPDE model (than a deterministic model), where the space fPDE describes fast uplift and the time fPDE captures the opposing periods.

3.1.6. Magma intrusion

Numerical models have been developed to simulate the emplacement of igneous bodies (sills/dikes), called the sill/dike intrusion model or magma intrusion model [94]. Magma emplacement velocities can vary dramatically. Some mantle rocks entrained within magma rise rapidly to the surface, with velocities of about 4 m/s [95]. Demouchy et al. [96] estimated that a xenolith can reach the surface from 60 to 70 km depth in several hours, a sparingly rapid rise, comparable to ascent rates for kimberlite magmas. Alternatively, other rocks may reside within magma chambers for extended periods of time, allowing partial or complete re-equilibration [97]. Hence, the time between two subsequent magma ascents can have a broad distribution, which might be better characterized by tempered one-sided stable density, as suggested by Cvetkovic [73], than a normal distribution or the standard stable density [4]. A tempered time fPDE therefore could be used to simulate the motion of magma or other igneous processes in the Earth's crust and lithospheric mantle. In addition, the magma temperature/cooling variability might also be simulated using the fractional-order Stefan model.

To summarize the discussion regarding internal Earth dynamics, regional and/or global convection within the core and mantle contains multi-scale dynamics occurring in a heterogeneous system, with limited system information and multiple unknown parameters, challenging traditional local models and motivating the application of fPDEs. Unlike the Newtonian fluids observed in the hydrosphere, here the fractional version of non-Newtonian flow models for outer core flow and magma intrusion and viscoelastic models for mantle convection will likely be needed. In addition, deep, internal Earth dynamics are correlated. For example, as previously discussed, outer core flow is linked with inner core rotation, and mantle motion drives continental drift, requiring coupled fPDE models. Because more information is available for shallower Earth processes than deeper dynamics, fractional calculus and fPDEs should first be developed for these shallow systems.

3.2. Large-scale Earth surface dynamics dominated by physical processes

Large-scale Earth surface processes have long been interpreted by numerical models, including the standard diffusion equation, advection/wave equation, and non-Newtonian flow equations (see, for example, Pelletier [98]). Typical large-scale Earth surface dynamics, especially geomorphic transport processes such as mass movement, sedimentary deposition, river networks, and Aeolian sand dune migration, can involve a wide spectrum of temporal and spatial scales and motivate the application of nonlocal transport theory. Indeed, watershed hydrologists have already suggested the fractional-order Eick's law as a possible alternative to the geomorphic transport law after the first STRESS (Stochastic TRansport and Emergent Scaling in Earth-Surface processes) workshop in 2007 [99], but the application of fPDEs for real-world geomorphic transport processes remains an open research question. The driving forces and dynamics for different geomorphic transport processes can differ significantly in different depositional environments, requiring systematic exploration for each process and specific treatment of the fPDE model.

Landscape evolution is a random process that is difficult to model using deterministic methods, due to the large number of processes and factors (such as fluvial erosion, slope processes, tectonic uplift, climate, and lithology) operating over a wide range of spatial and temporal scales [100]. For example, sedimentary deposits with time periods ranging from individual flooding events to geologic time are the result of erosional-depositional processes with a heavy-tail (i.e., power-law) distribution rate [101,102]. Efficient characterization of scale-dependent dynamics is one of the major advantages of fPDEs compared to standard models. For this reason, the fPDE models have been recommended by watershed hydrologists for bed-load transport in rivers [24,103], transport on hillslopes [22,104], and transport in river networks [99,105]. In the following, we discuss three important Earth surface processes in different systems that have not been focused on by the previous studies (Table 3).

3.2.1. Mass movement in the fluvial system

The most straightforward application of fractional-derivative models in solid Earth dynamics might be mass transport. Mass movement, also called mass wasting or landslide, refers to the downslope movement of mud, regolith (i.e., soil, sediment, and debris), rock, or snow/ice under gravity [106]. Mass movement plays a critical role in the rock cycle, affecting landscape evolution and producing stream valleys when mixed with running water. Five factors can induce mass movement: water, oversteepened slopes, removal of anchoring vegetation, earthquakes, and volcanic eruption, where earthquakes and excessive water (from a winter snow melt or a heavy rain storm) are the two most common triggers. Mass movement, however, can also occur without triggers. Slope materials may weaken over time or random, unpredictable events can occur. The variety of triggers, complex topography with multiscale heterogeneity, and potential interactions within moving materials can lead to high uncertainty in quantifying downslope mass movement when a deterministic model is used.

We classify subaerial mass movement into three groups, whose properties may guide the selection and development of fPDEs. We note that submarine landslides occur in oceans and therefore are not considered by this study. Group 1 exhibits extremely slow velocities, represented by (soil) creep caused by alternating expansion and contraction of the surface material due to freeze-thaw cycles that can last for years. Solifluction is a specific type of creep that is common in regions underlain by permafrost, and slump is another relatively slow moving of a mass of rock or unconsolidated material as a unit along a curved surface. These slow movements, which may represent sub-diffusive processes, may be quantified by the time fPDEs. Mass movements in Group 2 have extremely fast velocities, and this group includes avalanches and rockslides that can occur within seconds or minutes, which might generate super-diffusive motion and might be captured by the space fPDEs. Group 3 contains movement of material with variable speeds, including debris flow and mudflow, which can be mixtures of sub- and super-diffusion; therefore, this group requires mixed space and time fPDEs.

We select soil creep as an example to develop fPDE models. Soil creep is the most widespread (and also the least understood) erosion process on soil-mantled hillslopes [107]. Soil particles undergoing downslope creep are displaced in wetting-drying cycles over many years, a process analogous to mechanical dispersion. Field experiments by Heimsath et al. [107] using single-grain optical dating, showed that soil creep involves independent movement of mineral grains that can be intermittently reburied or eroded by overland flow upon reaching the surface. Therefore, the motion of creeping soil can be treated as independent and identically distributed (i.i.d.) random variables such as α-stable random noises, while the buried soil can be treated as immobile particles before they return to motion. This leads to a spatiotemporal fPDE, which is similar to the spatiotemporal fractional-derivative model proposed to simulate bed-load sediment transport in rivers that involves alternate transportation and storage [25].

FPDE models may also be developed for debris flow. Debris flows with destructive power can be one of the most hazardous consequences of rainfall, especially on burned hillslopes [108,109]. Storm-trigged debris flows in watersheds are best modeled as random processes because (1) they consist of a broad distribution of grain sizes, mixed and interacting with rapid-flow fluid; and (2) their dynamics depend on many different factors with multi-scale heterogeneity, such as hillslope morphology, flow properties, pore-fluid pressure, climate factors, and soil properties, which cannot be measured exhaustively at all relevant scales. Hence, stochastic models are needed to account for the randomness and uncertainty in quantifying the occurrence, yield, and dynamics of the multi-phase, gravity-driven debris flow. Most of the existing stochastic models have focused on landslide-trigged debris flows, including various physical-based models (i.e., mass-balance and momentum models) developed to simulate the dynamics of debris flows, such as the general two-phase model [110], the depth-averaged models [111,112], and the GIS-based cell model [113]. We can adopt the idea in Rengers et al.'s [114] process-based model to combine a rainfall-runoff model with a spatiotemporal fPDE model to capture the random dynamics in storm-trigged debris flow (a preliminary fPDE was developed for water flow along land surfaces at all scales by Zhang et al. [23]). Dynamics of the solid phase (i.e., weathered soil and fragmented rock) can be described by random displacement with random motion times, whose probability density functions will be defined and then validated using field observations of debris flow discharge (see, for example, Cannon and Gartner [115]).

In addition to the fPDE model (1), we can also apply the tempered one-sided stable density model to characterize the distributions of both motion size and trapping time for targets in mass movement [28,72,73]. A truncated Pareto distribution, whose summation can converge to the stable density, was also found to efficiently capture heavy-tailed geophysical distributions (such as the multiple-rate mass exchange between mobile water and immobile matrix in soils and aquifers) [23,116,117]. This shows the potential applicability of the tempered one-sided stable density function for quantifying mass movement dynamics, especially the extreme events with relatively low probabilities and large uncertainty.

3.2.2. Aeolian sand dune formation and movement in the Aeolian system

One fourth of the Earth's land surface is covered by arid regions, where desert sand dunes are the most common depositional landform. Dunes display a variety of shapes and sizes, depending on the character of the wind and the sand supply. There are five main types of dunes with different cross-beds, including (1) barchan dunes, with a crescent shape whose tips point downwind; (2) star dunes, consisting of overlapping crescent dunes formed by frequent shifts in wind direction; (3) transverse dunes, which are wave-like dunes formed when enough sand accumulates for the ground surface to be completely buried (but with only moderate winds); (4) parabolic dunes, formed when strong winds break through transverse dunes to make new dunes whose ends point upwind; and (5) longitudinal dunes, formed due to abundant sand and a strong, steady wind. Of these dunes, the crescent-shaped barchan dunes are found all over the world and have been studied extensively. Isolated barchan dunes can be 9–30 m high and 370 m wide, and they can migrate with the wind at a rate varying from 1 to 100 m per year.

Quantification of sand dune migration has critical implications for the ecosystem, economy, and society. Numerical simulation of Aeolian dune dynamics using physical models, however, remains a challenge after more than four decades of work. This challenge is due to the complex interactions between sand dune morphology, turbulent wind flow, and sediment transport that exhibit multi-scale heterogeneity (see, for example, Livingstone et al. [118]). Interaction between dunes may also affect dune transport (including movement and growth) since sand dunes frequently propagate as a group and form arid sand seas.

Since the 1970s, various physical models have been developed, which mostly focus on the dynamics of barchan dunes. The early analytical approach was developed by Jackson and Hunt [119] and improved by others (e.g., Wippermann and Gross [120]; Weng et al. [121]) to obtain the analytical expression of wind-induced transport for an isolated dune. A heuristic approach was proposed by Zeman and Jensen [122] and applied further by Sauermann et al. [123] to model airflow over a dune. A continuum saltation model, based on (standard) momentum conservation, was also developed [124,125], assuming equilibrium in sand flux. A popular linear expansion model was then developed by Andreotti et al. [126], Lima et al. [127], Schwämmle and Herrmann [128], and Hersen [129] to simulate barchan shape and migration patterns. Computational fluid dynamic (CFD) models, which are likely the most reliable and detailed physical models, were applied to describe flow over Aeolian dunes [130] (for transverse dunes). However, a detailed distribution of turbulent wind velocity is required, challenging the applicability of CFD models and motivating the application of fPDE models for grouped barchans. Recently, a cellular automaton model was proposed to simulate vertical sorting in granular mixtures (i.e., aggregating the small-scale, individual grain motions and saltation) for steady unidirectional flow conditions [131], a specific wind condition with limited applicability in the field. Advanced physical models are still needed to understand the nature of sand dune dynamics, with additional help from recently developed and significantly enhanced field monitoring techniques.

Complex dynamics and random nature in dune development motivate the application of stochastic models. We expect that the introduction of fractional calculus in Aeolian dune simulations may enhance standard models in at least four ways. First, fractional derivative terms can capture the impact of sub-grid variation in wind properties (speed and direction) and sand heterogeneity on dune dynamics, which cannot be mapped exhaustively by standard models [35]. Second, turbulent wind (with an upper limit in velocity) can cause complex sand dynamics, whose motion can be (better) described by (tempered) Lévy motion related to fractional derivative models. Third, sand movement can have memory in space (especially for erosion on the windward side) and time (when buried below the surface or deposited on the leeward side), which can be efficiently captured by space and time fractional derivative models. The buried sand particle eventually returns to surface and migrates again, after wind removes the top layer, leading to a finite, maximum trapping time. Fourth, if sand dune evolution is not a simple equilibrium system, but rather a kinetic process with varying total mass, then its dynamics can be captured by the kinetic, fractional-in-time derivative model. It is also noteworthy that the fPDE may require a space-dependent fractional index, leading to the variable-index fPDE discussed in Section 4.3. For example, kinetics of sand at the windward side may require a spatiotemporal fractional derivative term, due to both erosion and fast movement of sand, while the leeward side of dunes may require a time fractional derivative term due to random retention of sand particles.

3.2.3. Glacial erosional–depositional processes

Subglacial erosion is important for the present topography of Earth's surface, although the mechanisms driving subglacial erosion are not very clear [132]. There are two major forms of erosion: abrasion and quarrying. Abrasion can polish the surface of the underlying rock and generate glacial striations. Quarrying includes both plucking and bulldozing impacts (i.e., lifting and pushing of rocks), which were modeled recently by Ugelvig et al. [132]. Many factors can affect the rate of subglacial erosion. For example, hydrologic conditions (including drainage efficiency, which regulates the effective pressure, and surface slope) as well as fracture density and orientation of the underlying bedrock can affect the quarrying rate [132].

Local models have been used to describe glacial erosion. In most glacial landscape evolution models, the erosion law takes the form [133-135]:

$$E = au^b, \tag{4}$$

where E is the glacial erosion rate, u is the basal sliding speed, and a and b are constants, where $b = 1$ is typically assumed to reach a simple linear relationship between erosion and sliding. This law (4) is valid only at the local scale. Another model related to glaciers, the glacial isostatic adjustment model, is commonly used to evaluate the impact of mass or thickness change of ice sheets on the rise of land mass. In this model, the sea-level change (S) is usually modeled by [136]:

$$S(\theta, \lambda, t) = C(\theta, \lambda, t) \times \left[\int_{-\infty}^{t} dt' \iint_{\Omega} d\Omega' L(\theta', \lambda', t') G(\nu, t - t') + \frac{\Delta\Phi(t)}{g} \right] \tag{5}$$

where θ and λ denote the latitude and longitude, respectively; C denotes the ocean function (=1 for ocean and 0 for continent); L is the surface mass load per unit area; G denotes the kernel; and the last term on the right-hand side (RHS) of (5) is added for mass conservation purposes. A nonlocal model may be needed to generalize the simple relationship (4) to capture large-scale subglacial erosion significantly affected by the small-scale variation of hydrology conditions and rock properties. It is also interesting to replace the local kernel in (5) by a nonlocal kernel, to capture sea-level change due to the nonlocal impact of controlling factors.

Numerical modeling of glacial depositional processes remains a historical challenge. Glacial motion, which is important for the rock cycle and hydrologic cycle, occurs mainly as basal sliding (where the entire glacier slides over its bed), plastic flow within the ice (due to plastic deformation), and glacial surges (i.e., movements of large sections of ice up to 100 times faster than normal). Glacial motion leads to two types of deposits: (1) landforms made of glacial till (which are sediments deposited directly by glacial ice) such as moraines, and (2) landforms made of stratified drift (layers of sand and gravel accumulated in braided stream channels), including outwash plains and ice-contact deposits, such as kame and esker. Simulation of glacial deposits is not trivial. For example, moraine evolution is affected by debris concentration, ice melt-rate, and debris flux [137], which vary randomly in space and/or time and are difficult to measure in the field. Hence, stochastic models such as fPDEs may be preferred to describe the glacial depositional processes.

To summarize, large-scale Earth surface dynamics can occur in different systems and are driven by various forces, requiring different fPDEs (or fPDEs with different memory functions). Particularly, the response of these dynamics to externally-driven forces and internal interactions may lead to complex memory functions expressed by fPDEs (2). In addition, poor predictability is one of the major shortcomings of fPDEs (see further discussion in Section 4.1), but the Earth surface dynamics mentioned above, except for the elusive glacial erosion and deposition, may improve model predictability. With a wide range of observed information (such as remote sensing and geophysical survey data) and enhanced monitoring techniques, there is an unprecedented opportunity to build a (at least partially) predictive fPDE model. For example, memory kernels in the generalized stochastic model (2) can be tested using observed debris flow yields, whose potential final format (i.e., from power law to tempered one-sided stable density) might be linked with the most pertinent, observable items (such as the reach length and width of entrainment/deposition, watershed size, lithology, precipitation depth, duration and overall shape, and flood volume, runoff coefficient and peak flows).

3.3. Small vertical-scale earth surface dynamics

Small-scale surface processes (usually with a growth/erosion direction perpendicular to the local surface), such as crystal growth, rock/mineral weathering, and pedogenesis, are major research targets for mineralogists, soil scientists, and geomorphologists. Under real-world geological conditions, reliably and efficiently modeling these dynamics remains a challenge.

3.3.1. Crystal growth (nanometer to millimeter scale)

Mineral crystal growth is important for all geological processes, including the formation of cements in sedimentary rocks, the filling of fractures to form veins, recrystallizing rocks by solid-state processes during metamorphism, and growing crystals from magma to form igneous rocks. The kinetics of crystal growth can be affected by many factors, including liquid properties (i.e., level of supersaturation and deposition rate), crystallographic anisotropy, physical properties, the crystal's surface morphology (i.e., free energy barriers, segregation of impurities, and the nucleation and spreading of clusters at the crystal surface), thermal fluctuations, and/or evaporation rate.

Tremendous efforts have been made to quantify crystal growth using mathematical models, particularly including the following four common models. First, the well-known, simplified Frank's model [138] shows that the velocity of the crystal surface propagation is proportional to the local surface orientation, which is strongly related to substrate geometry rather than to physics. Second, the simplest mathematical description for a perfect impurity-free crystal is the solid-on-solid (SOS) model, which assumes an exponentially-declined deposition rate and multiple effective evaporation rates in a simple mass balance format (see Weeks and Gilmer [139] (Eq. (3.5)) for the dynamics of crystal growth). Third, the highly-cited Burton-Cabrera-Frank (BCF) model describes a crystal's density evolution using the following PDE [140]:

$$\frac{\partial \rho(z,t)}{\partial t} = D_s \frac{\partial^2 \rho(z,t)}{\partial z^2} - \tau \rho(z,t) + F, \tag{6}$$

where z is the direction perpendicular to the steps, $\rho(z, t)$ denotes the adatom density, D_s is the microscopic surface diffusion constant of adatoms, τ defines the evaporation rate, and F is the adatom deposition rate. The BCF model (6) was built upon the standard mass balance law, where normal diffusion for adatoms was assumed.

Fourth, crystal growth can also be modeled by the well-known Kardar–Parisi–Zhang (KPZ) equation, a non-linear stochastic PDE describing the temporal change of the height $h(\vec{x},t)$ of the crystal surface at location $\vec{x}$ and time t [141,142]:

$$\frac{\partial h(\vec{x},t)}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(\vec{x},t), \tag{7}$$

where $\nu > 0$ is a constant (surface tension), λ is the kinetic coefficient, and $\eta(\vec{x},t)$ is the Gaussian white noise (representing, for example, fluctuations of beam intensity) with a zero mean and the following variance:

$$\langle \eta(\vec{x},t)\eta(\vec{x}',t')\rangle = 2D\delta^d(\vec{x}-\vec{x}')\delta^d(t-t') \tag{8}$$

Here, D denotes a parameter and d denotes its dimension. The first term on the RHS of (7) describes relaxation of the interface, and the second term on the RHS of (7) is the lowest-order nonlinear term appearing in the interface growth equation (i.e., Taylor expansion of the surface growth rate; see Kardar et al. [141]). The KPZ Eq. (7) is the general theory of surface growth models, such as the Eden model (which describes the growth of specific types of clusters growing by random accumulation), the surface fractal model (such as fractal landscape), and the SOS model mentioned above. The vector KPZ model (7) reduces to the following one-dimensional version:

$$\frac{\partial h(x,t)}{\partial t} = \nu \frac{\partial^2 h(x,t)}{\partial x^2} + \frac{\lambda}{2}\left[\frac{\partial h(x,t)}{\partial x}\right]^2 + \eta(x,t), \tag{9}$$

where the surface grows in a normal direction (perpendicular to the space x axis), $\partial h(x, t)/\partial x$ denotes the surface slope, and the second term on the RHS of (9) denotes the nonlinearity coming from this simple geometric effect.

There are three primary motivations to apply a stochastic model, such as the generalized fPDE (2), to quantify crystal growth kinetics under natural geological conditions. First, crystal growth kinetics can be diffusion-controlled, especially under high supersaturation conditions (see, for example, Collins and Levine [143]). There are multiple diffusive stages related directly to crystal growth and dissolution. For a crystal to grow, atoms and energy need to diffuse up to the substrate surface; while for a crystal to dissolve, atoms must be carried away [142]. Impurities, which can be present in natural conditions, also diffuse to the surface to facilitate crystal growth [144]. Hence, crystal growth is a nonlocal process [142]. Considering the natural heterogeneity in rock property and liquid, it is most likely that some of the diffusion dynamics can deviate from Fick's diffusive law and significantly affect the crystal growth rate. Second, atoms undergo random walking on the crystal surface before they can merge, and Brownian motion has been assumed by standard models. It is a logical expectation that (tempered) Lévy motion should replace Brownian motion for random atom jumps under natural geological conditions. Third, crystal growth might not always be continuous, but rather it may be mixed with episodic fast growth and subsequent periods of dissolution. For example, episodic flow of high-pressure water in fault zones can affect the dynamics of crystal growth. Seismic pumping due to shallow earthquakes provides an explanation for the textures of hydrothermal vein deposits associated with ancient faults, which almost invariably indicate that mineralization was episodic [145]. Hence, crystal growth might be approximated by a CTRW process with independent growth (or precipitation) and waiting (or dissolution) periods, a process which can be described by the fPDE (2).

Indeed, various fractional versions of the KPZ model (7) have been proposed, although none of them have been used for the actual crystal growth process yet. For example, Katzav [146] proposed the following fractal KPZ equation for growing surfaces with anomalous diffusion:

$$\frac{\partial h(\vec{x},t)}{\partial t} = \nu(\nabla_\alpha h) + \frac{\lambda}{2}(\nabla h)^2 + \eta(\vec{x},t), \tag{10}$$

where the operator $\Delta_\alpha \equiv -(-\Delta)^{\alpha/2}(1 < \alpha \le 2)$ is the fractional Laplacian. The same expansion was used by Xia et al. [147], where the standard second-order space derivative was replaced directly by a space fractional derivative. Recently, Hoshino [148] replaced the white noise in (7) by a fractional derivative term:

$$\frac{\partial h(\vec{x},t)}{\partial t} = \nu\left(\nabla^2 h\right) + \frac{\lambda}{2}(\nabla h)^2 + \frac{\partial^\gamma}{\partial t^\gamma}\eta(\vec{x},t), \tag{11}$$

where γ is the same as the time index used in model (1). A space-fractional KPZ model was proposed and solved numerically by Xia et al. [147], and a time-fractional KPZ model and its solution were analyzed by Abdellaoui and Peral [149].

The above models provide the preliminary fPDEs to quantify crystal growth of minerals. By combining the time and space fractional derivative terms introduced in these previous studies, one obtains the following fPDE (in one-dimension):

$$\frac{\partial^\gamma h(x,t)}{\partial t^\gamma} = \nu\frac{\partial^\alpha h(x,t)}{\partial x^\alpha} + \frac{\lambda}{2}\left[\frac{\partial h(x,t)}{\partial x}\right]^2 + \eta(x,t), \tag{12}$$

which is the fractional version of the KPZ model (10). Model (12) can be solved numerically, for example, using the finite-difference method proposed by Xia et al. [147]. Further extension of (12) following the generalized fPDE (2) (plus the nonlinear term to capture the geometric effect) can be explored to capture the episodic growth and dissolution processes. It is also noteworthy that other natural growth processes, such as tree ring growth (where the ring width is affected by temperature, rainfall, and humidity), shell ring growth (affected by sea-surface elevation, supply of nutrient and calcite, salinity, and temperature), and speleothem growth (affected by precipitation and CO_2 concentration), share similar dynamics and may benefit from the development of the above stochastic models.

3.3.2. Rock/mineral weathering (nanometer to centimeter scale perpendicular to the surface)

Weathering provides the material for sedimentary rock formation and is important for numerous geochemical cycles involving the lithosphere, hydrosphere, and atmosphere. The weathering processes can be driven by complex physical, chemical, and biological factors involving plant and animal life, atmosphere, and water [150-152]. Specifically, changing environmental conditions (including precipitation, snow/ice, temperature, humidity, exposure, wind speed and direction, and biological activities) and tectonic events can result in a spatial-scale dependent weathering rate, a time-scale dependent weathering response, and time-scale sensitive weathering kinetics (i.e., episodic manner in transient weathering), making the deterministic study of weathering difficult. Some small-scale properties, such as the mineral reactive surface area, can also affect chemical weathering rates [153]. Although vertical weathering only occurs at mineral surfaces and covers the nanometer to centimeter scale, the horizontal spatial scale for weathering can extend to entire plates [154]. The geological time scale for weathering increases from thousands of years (such as the response of weathering to temperature perturbations) to tens of millions of years (such as soil development in the tropics along a gentle slope) [155]. Due to the scale dependence and multiple elusive controlling factors, weathering rates measured in the laboratory can be significantly higher than field measurements, which is similar to the well-known trend for the diffusion-limited chemical reaction rate observed by hydrogeologists (see the review by Dentz et al. [156]). It is also noteworthy that physical weathering (or physical denudation) mainly depends on lithology, regional relief, runoff, and other environmental factors, which are relatively less complex than those controlling chemical weathering. Hence, in the following, we focus on chemical weathering.

Various models have been developed to calculate chemical weathering rates in the field. For example, Maher et al. [157] applied a multi-component reactive transport model (CrunchFlow) to interpret mineral precipitation/dissolution rates. Maher [158] also linked the global bulk weathering rate to the fluid residence time (see their Eqs. (6)–(8)) which has a wide distribution. A similar steady-state weathering model was applied by Hren et al. [159] to describe the relative impact of reaction kinetics and rock supply on weathering rates. Maher and Chamberlain [160] also treated the weathering rate as a function of the tectonic regime.

Chemical weathering rates at large scales (i.e., watershed to global) have been typically analyzed with flux concentrations of solute observed in streams, assuming a simple linear relationship between weathering rates and major controlling factor(s). This led to steady-state partitioning models, calculating silicate weathering reactions with both dissolved and solid weathering products [161]:

$$W = \frac{q_d}{q_w} \tag{13a}$$

$$W_C = \frac{C_d q_d}{C_w q_w} \tag{13b}$$

where W denotes the weathering rate for the fraction of bedrock that erodes in solution, W_C is the weathering rate for the fraction of silicate dissolved from eroding bedrock, q_w denotes the flux of weathered bedrock silicate, q_d denotes the flux of the dissolved chemical, and C refers to concentrations with respect to the mass of solid material (C_w) or the dissolved material (C_d).

In addition, the PROFILE model proposed by Sverdrup and Warfvinge [162,163] and applied widely by others [164–166] is a steady-state soil chemistry model that can calculate the rate of chemical weathering of soil minerals using the transition state theory. The weathering rate of silicate minerals in soil was assumed to be proportional to the exposed surface area of the mineral, the soil moisture saturation, and the chemical driving force. For example, the steady-state weathering rate for organic ligands was calculated by Sverdrup [167]:

$$R = A_s C_s Q \tag{14}$$

where R denotes the weathering (reaction) rate, A_s denotes the area of active surface (i.e., the mineral surface that is wet and in contact with the soil solution), C_s denotes the contents in the surface, and Q is the chemical rate per unit surface area. The steady-state rate of cation release by mineral weathering could also be simplified as [168]:

$$R = \frac{K_B[B]^n}{f_B} \tag{15}$$

where K_B is the rate coefficient for cation B, f_B is the retardation factor, $[B]$ is the ion concentration, and n is the reaction order. The above calculation of weathering rate contains high uncertainty, due, for example, to the unrealistic constraints imposed by the use of the surface area equation (note that some parameters in the model, such as the surface area fraction, are almost impossible to measure), as shown by Hodson et al. [168].

Weathering due to chemical transformations, combined with physical deformations, was calculated by the steady-state chemical mass-balance model proposed by Brimhall and collaborators [169–172]. This simple model calculates the change of rock/soil material thickness ε [dimensionless]:

$$\varepsilon = \frac{\rho_r}{\rho_s}\frac{C_{i,r}}{C_{i,s}} - 1, \tag{16}$$

where ρ_s and ρ_r $[ML^{-3}]$ are the density of soil and rock, respectively; and C_i $[MM^{-1}]$ is mass concentration of the immobile element in rock ($C_{i,r}$) or soil ($C_{i,s}$). The sign of ε (positive or negative) represents variation of the soil profile (dilation or collapse).

The above models have two historical challenges. First, these steady-state models assume that the statistical properties of dynamics processes remain stable [154]. This ideal steady state may never exist in real-world geomorphology. This is because tectonic and climate conditions constantly change with possibly nonstationary statistics. Particularly, chemical weathering requires the presence of water. Storms in acidic areas can cause significant and rapid weathering, while cracking can also enhance weathering. Hence, chemical weathering in the field may actually be a random process with a mix of broadly distributed fast and slow periods. Second, whether the deterministic models can capture scale-dependent, complex weathering rates remains unclear. The rate of chemical weathering in the field, measured by chemical mass balance, isotopes, and element depletion, can vary by orders of magnitudes (see Langan et al. [173]). Colman [174] reviewed various studies of rock weathering and suggested that the rate of weathering (R) decreases with time and that the weathering rate can be approximated as a logarithmic time function: $R \propto \ln(t)$. White and Brantley [175] found that the average silicate weathering rate R decreases as a power-law time function: $R = 3.1 \times 10^{-13}\ t^{-0.61}$, likely due to the combined impact of intrinsic processes (such as intrinsic surface area, which increases with the duration of weathering, progressive depletion of energetically reactive surfaces, and accumulation of leached layers and secondary precipitates) and extrinsic controls (including low permeability, high mineral/fluid ratios, and increased solute concentrations), which cannot be measured exclusively and quantified by deterministic models.

The fPDE may be developed as an alternative to the above steady-state models to capture the transient weathering rate with scale dependency, random episodicity, and strong perturbation. Process-based models of weathering would be ideal, while deterministic models that can characterize the complex impact of chemical, physical, and biological processes on weathering will remain largely empirical [154]. This challenge motivates the application of stochastic models, especially the tempered fPDEs, which are efficient for both space- and time-scale dependent dynamics [41]. For example, the strong perturbation of weathering rate (especially with fast rates due to cracks and/or storms) may be described by a space-nonlocal term, and the episodicity in weathering can be explained using the concept of weathering periods separated by dormant stages (which can exhibit a heavy-tailed distribution since weathering occurs on a geological time scale).

3.3.3. Pedogenesis (centimeter to meter scale)

Pedogenesis involves the genesis, formation, development, and evolution of a soil affected by interconnected physical, chemical, and biological factors. As such, it is critical to all forms of life. These complex processes have been interpreted for decades by soil scientists and geomorphologists using various process-based mechanistic models (see, for example, Minasny et al. [176]). Mechanistic models of soil development in a landscape usually formulate a continuity equation to capture the change in soil properties over time as a function of material transport. One of the simplest mechanistic models for soil development takes the form [176,177]:

$$\frac{\partial H}{\partial t} = \frac{\rho_r}{\rho_s}\frac{\partial e}{\partial t} - \nabla q_s, \tag{17}$$

where H $[L]$ is soil thickness, e $[L]$ is the boundary between the soil and bedrock, t $[T]$ is time, q_s $[L^3\ T^{-1}]$ is material flux, and ∇ is a partial derivative vector. This model forms the bases of landscape evolution models. The derivative in the first term on the RHS of model (17), $\partial e/\partial t$, describes the rate of soil production, which can be related to the rate of rock weathering discussed above [176].

To simulate soil evolution, Minasny and McBratney [178] developed a mass-balance formula by considering the soil production and transport (also see Minasny et al. [176]):

$$\frac{\partial C}{\partial t} = I + D_c\frac{\partial^2 C}{\partial z^2} - kC - q_C, \tag{18}$$

where C $[LL^{-1}]$ denotes the concentration (such as the soil organic carbon concentration), I $(=\partial e/\partial t)$ is the soil production rate, D_C $[L^2T^{-1}]$ is the constant diffusion coefficient (describing the vertical mixing of organic materials by soil fauna), k denotes the loss rate (such as the rate constant of decomposition), and q_C is the transport of soil along the hillslope, which can be modeled as a simple diffusion process. The above model can simulate the evolution and distribution of soil thickness and organic carbon concentration in a landscape.

Fractional calculus might be applied to enhance the model capability for soil evolution. For example, the constant diffusion coefficient assumed by model (18) cannot capture vertical heterogeneous mixing, and the lateral transport of soil materials along a regional-scale slope does not always follow normal diffusion, perhaps due to topography. A fractional version of the comprehensive soil evolution model can be built by extending the local diffusion in the above model to nonlocal, anomalous diffusion. In addition, the possibly slow evolution of soil organic carbon concentration or long-term erosion processes can be conveniently captured by replacing the integer-order temporal derivative on the left-hand side of (18) by a time-fractional derivative. Hence, the general fPDE model (2) might be used to develop a stochastic soil production and transport model to quantify pedogenesis.

To summarize, the small vertical-scale Earth surface dynamics described above can be affected by mixed geochemical and physical factors, and they can exhibit similar patterns, such as random episodicity and diffusion-related kinetics. They all require the interaction between solid (rock or minerals) and water. It is therefore not surprising that they were previously described by similar PDEs built upon mass conservation. For example, the soil production and transport model (18) is analogous to the BCF model (6) describing crystal growth, which has the same limitation in capturing non-Fickian diffusion. Hence, we can focus on the fractional-order KPZ model (in both space and time) by extending the fPDE model (2) to describe crystal growth of minerals in the field. The resultant fPDE with simplification (i.e., removing the nonlinear term) can be applied to capture transient rock/mineral weathering as well as soil production and transport.

4. Challenges and future development of fPDEs in quantifying geological dynamics

Historical challenges, such as the poor predictability of model parameters and the unclear mathematical specification of bounded fractional diffusion, can hinder practical applications for fPDEs in geological dynamic processes. Other possible reasons for the limited application of stochastic theories in hydrologic sciences were identified by multiple groups of hydrologists (see, for example, the recent debate about the failure of stochastic hydrogeologic approaches in capturing reactive transport in real-world aquifers [42,43,48,179,180]). Opinions are also found in the 2004 forum [181], where nine eminent researchers identified the following reasons preventing stochastic hydrology approaches from becoming routine hydrological modeling tools: (1) sociological elements including the lack of handy tools and communication, and potential conflicts [182]; (2) the time gap between research advancements and application, and the lack of data and well-established tools [183]; (3) the lack of interest by clients in model uncertainty analysis, and the actual hydrogeological, technical, and social uncertainties [184]; (4) technical limitations in reflecting real-world conditions, the failure to communicate, interdisciplinary demanding, and debatable assumptions such as stationarity and ergodicity [185]; (5) limited measurement capability and non-stationary natural sediments [186]; (6) the challenge of data collection and aquifer parameter estimation, the problematic assumption of ergodicity, and the lack of software and education [187]; (7) the lack of multidisciplinary efforts [188]; (8) the lack of education, and the lack of interest from regulators in uncertainty [189]; and (9) most stochastic models being too simple to be relevant to real problems [190]. To summarize, the lack of aquifer information and the failure to capture real-world conditions (such as nonstationary aquifers) were the most significant criticisms by the hydrogeologic community for stochastic approaches. Here, we discuss the gap between the fPDEs and real-world practical applications, by focusing on the major technical challenges associated with the fPDEs and proposing possible solutions when applying fractional calculus to capture complex dynamics in the Earth systems discussed above.

4.1. Parameter predictability

It is difficult to predict complex dynamics in either the hydrosphere or the solid Earth using nonlocal transport models, because of the unknown quantitative relationship between model parameters and medium properties (or the other major controlling factors). A few numerical tools are available to fit the model parameters given measurements (such as pollutant breakthrough curves or BTCs in the hydrosphere), including the particle-tracking approach proposed by Chakraborty et al. [191], the nonlinear regression method proposed by Lim et al. [192], and the local and global optimization scheme proposed by Kelly et al. [193]. Model prediction, however, is much more difficult and practically important than the fitting exercise. As discussed above, it is plausible (and sometimes necessary) to propose a fractional-order Fick's law of diffusion, Newton's law of viscosity, or Fourier's law of heat conduction, and to introduce heavy-tailed memory kernels in spatiotemporal convolution to account for the time rate change of mass, momentum, or energy. Prediction of the proposed nonlocal parameters in real-world applications for geological media, however, has never been trivial. In addition, the best-fit parameters might not be unique for a given BTC if multiple parameters control similar behavior of transport, such as the late-time tailing in the BTC.

The recent work of Zhang et al. [15] using extensive Monte Carlo simulations provides one example of how to build a predictive fPDE for pollutant transport through regional-scale fluvial aquifer/aquitard settings when the flow remains steady state. Particularly, the two time-nonlocal parameters in model (1), which control pollutant retention in immobile domains, including the time index γ and the time truncation parameter λ_T, can be estimated given the volume fraction of low-permeability floodplain deposits classified by thickness that can be gleaned from detailed well logs, outcrops, and/or geophysical surveys. Extra caution is needed when approximating the effective velocity and dispersion coefficient in the fPDE (1), which in this example, describes pollutant displacement in mobile time that could not be predicted accurately based on measurable lithology, since the exact pathway for pollutants is difficult to predict even given the spatial distribution of lithology or local velocity distributions.

To enhance the fPDE model predictability, extensive field/laboratory experiments and Monte Carlo simulations are needed to link model parameters to statistics of major properties of geological media and natural triggers. Field monitoring techniques, such as remote sensing, geophysical survey, and seismic wave survey, can be applied to enhance model predictability. Novel inverse modeling approaches can also be helpful to directly calculate the memory kernels in model (2) using observed dynamics.

4.2. Fractional diffusion in bounded domains

Dynamic processes in the Earth system are typically bounded in geological space and time. Previous applications of fPDEs in geology, especially the hydrologic sciences, however, have been limited to unbounded spatial domains, because the mathematically-correct specification of fractional differential equations on a bounded domain remains a historical challenge. It is not trivial to define boundary conditions for a fPDE, because fractional derivatives are nonlocal operators, and the nonlocal boundary condition extends beyond the boundary. An arbitrarily defined, spatially-nonlocal, fractional-order boundary condition may lead to an ill-posed fPDE.

Recently, several researchers have focused on bounded fractional diffusion. For example, Baeumer et al. [194] defined the fPDE with a specific reflective boundary in a semi-finite, one-dimensional domain:

$$\frac{\partial f(x,t)}{\partial t} = \frac{\partial^{\alpha} f(x,t)}{\partial (-x)^{\alpha}} \tag{19a}$$

$$f(x,t)|_{t=0} = \delta(x - x_0) \tag{19b}$$

$$\left. \frac{\partial^{\alpha-1} f(x,t)}{\partial (-x)^{\alpha-1}} \right|_{x=L} = 0 \tag{19c}$$

$$f(x,t)|_{x=+\infty} = 0, \tag{19d}$$

so that no external, nonlocal diffusive flux can recharge via the upstream boundary and affect the internal super-diffusive dynamics, keeping the boundary value problem well-posed. Defterli et al. [195] used the recently developed theory of nonlocal diffusion to identify a well-posed fPDE with an absorbing boundary. Sankaranarayanan [196] worked on the one-sided fADE on the interval (0, 1) and defined the appropriate reflecting and absorbing boundary conditions (by assuming zero density outside the model domain, to simplify Grünwald-type approximations). The mathematically-correct specification of a general fPDE on a bounded domain with generalized, nonzero-value Dirichlet, Neumann, or mixed Robin boundary conditions, however, remains obscure, and therefore, whether there exists a unique solution depending continuously on the initial data for the general bounded fractional diffusion model remains unclear.

To obtain an applicable boundary value problem for the hydrologic community, Zhang et al. [197] proposed specific nonlocal boundary conditions (with both zero and nonzero-value Dirichlet, Neumann, and Robin boundary conditions) for the fADEs and developed particle tracking codes to solve these specific fractional boundary value problems. Results showed that the sign of the Riemann–Liouville fractional derivative (capturing nonzero-value spatial-nonlocal boundary conditions with directional super-diffusion) should remain consistent with the sign of the fractional-diffusive flux term in the fADEs, and non-traditional schemes must be used in the Lagrangian solver for the reflective boundary so that the mathematical problem (e.g., the form of the fADE) remains unchanged. Tremendous efforts are still needed to interpret the mathematical problems and physical meanings for bounded fPDEs before we can reliably quantify bounded non-Fickian dynamics in the Earth system.

4.3. Spatially and temporally nonstationary transport

FPDEs are the scaling limit of stochastic processes with random-walking particles undergoing Lévy motion, and therefore, the fPDE models with constant parameters can be used for a system with stationary heterogeneity where the statistics of target dynamics remain stable. The assumption of stationarity has never been systematically checked for real-world geological media, likely due to the technical difficulty and prohibitive burden. Spatial non-stationarity with heterogeneity evolution, due to the change of large-scale tectonic/environmental conditions and/or sediment supply, however, is not uncommon in real-world depositional systems, violating the ergodicity assumption and challenging the application of fPDEs with constant parameters, especially the constant time/space index, which is the upscaling parameter for the statistically homogeneous medium.

For spatially nonstationary systems, both the time memory function (f) and the kernel (g) for diffusive jumps in the generalized fPDE (2) can be space dependent, to capture anomalous scaling with the travel distance. Berkowitz et al. [198] also suggested a space-dependent memory function in their continuous time random walk framework, although the geological delineation of representative zones with characteristic stationarity remains unclear. Anomalous scaling due to spatial non-stationarity, therefore, may be captured by the variable-order fPDEs [e.g., 199–202], distributed-order fPDEs [203–208], or their mixture [209]. In hydrologic sciences, the variable-order fPDE was firstly applied by Zhang et al. [25] to capture observed large-scale bed-load sediment transport in rivers and by Sun et al. [210] to simulate contaminant transport observed in porous and fractured aquifers. Further hydrological applications are needed to reveal the relationship between the evolution of natural geological media and index variation in fPDEs, in addition to the exact representative scale of the upscaled, fPDE model.

To further challenge the application of single-index fPDEs, spatially-stationary media can invoke temporally nonstationary transport behavior. The impact of non-stationarity can also occur in time in statistically homogeneous media, requiring a time-dependent index in the fractional derivative. For example, under specific hydraulic conditions, such as transient flow, changes between stress periods, boundary conditions and/or types, or the reverse of flow direction (due, for example, to the pump-and-treat process during groundwater contamination remediation), behaviors of anomalous transport may change with time, as proposed by Fogg and Zhang [180]. This was partially observed by Fogg et al. [211] and Zhang et al. [46]. Parameters in fPDE (1) might be time-dependent because the pathways for water and chemicals now change with time due to the temporal fluctuation of magnitude and/or direction of flow velocity. More generally, model parameters might be functions of time, leading to a variable-order fPDE with a time-dependent index [210] or a distributed-order fPDE where the waiting times between particle jumps distribute as a mixture of power laws [211].

It is important to distinguish transient diffusion caused by local variation of system properties and non-stationary evolution of system heterogeneity, both of which can cause temporal- and/or spatial-scaling of anomalous diffusion. Single-order fPDEs with variable velocity and dispersion coefficient [12] or the single-order fPDEs with a tempered stable density [41], which are favored by hydrologic modelers due to fewer parameters than the multi-order fPDEs, should be used to describe spatiotemporal-dependent diffusion in stationary geological media with local variation of geological properties, such as the local fluctuation of aquifer/aquitard material proportions or different regions of an ancient meandering river, like the one observed at the well-studied MADE test site [212,213]. However, for strong variation of anomalous diffusion, such as the apparent and quick transfer from sub-diffusion to super-diffusion (and vice versa), which cannot be explained reasonably by local variation of medium properties, the variable-order fPDE might be a better choice.

4.4. Incorporating geologic information in fPDEs

The lack of incorporation of geological characteristics, especially critical geologic architecture controlling mass/momentum/energy dynamics, in stochastic hydrogeology has been identified by various hydrologists as the major reason for the gap between stochastic approaches and practical applications (see the review by Rajaram [43]). To capture regional-scale dynamics occurring in geologic media, major geologic and physical architecture (that can cause non-Fickian dynamics) should be well characterized in the model, including, especially, spatially-interconnected preferential pathways (such as ancient channels in alluvial deposits) for mass/momentum/energy and the surrounding “stagnant” zones (such as the floodplain deposits), which retard the target dynamics. However, the fPDE, as a parsimonious, upscaling model, was designed to capture super-diffusion and sub-diffusion without the necessity to map detailed medium heterogeneity. The dilemma is that the fPDE works the best for a transport distance covering all representative heterogeneity, or approaching the asymptotic state. In a real-world problem, such as a typical contaminant plume observed in clastic sedimentary deposits, the plume longitudinal length is usually on the order of $10^2 \sim 10^3$ m [180], and hence, the majority of pollutants may only sample part of the medium heterogeneity, violating the upscaling assumption of fPDEs. For example, at the MADE test site, the tracer (bromide and tritium) plume extended only $\sim$300 m downstream in one year, where the tracers were mainly located in the connected gravel and sand deposits [214]. Similar plume size and transport paths could also be found for the other natural gradient tracer test sites [180]. This pre-asymptotic transport due to short travel distance is the opposite of long distance, nonstationary transport discussed in the previous section. In this case, local variations of geologic architecture need to be incorporated in the model to capture the nuance of pre-asymptotic transport.

One solution is to develop a pre-asymptotic nonlocal model, such as the tempered fPDE [41], conditioning on local geologic properties, such as the field-measured flow velocity, porosity, lithology, soil moisture, or any other information using geology, hydrogeology, geophysical survey, and/or remote sensing. Some preliminary tests were presented by Zhang et al. [28], and further real-world applications are needed. The balance between sub-grid resolution of medium heterogeneity (such as flow velocity and topography) and fractional diffusion (in both space and time) also needs to be defined to address the above issue.

4.5. New fPDEs required for additional functionality

New fPDEs may be required to model complex dynamics in the solid Earth. For example, mudflow contains interacting water and solids, whose movement affects each other. A fractional-order, multi-phase-coupled physical model is therefore preferred. In addition, non-Newtonian behavior in the outer core and magma chambers, and viscoelastic flow associated with mantle convection, require the development and application of fractional-order constitutive equations (see, for example, Bagley and Torvik [215] and Mainardi [216]) for geological dynamics.

5. Conclusion

Effective simulation of geological dynamics in both the solid Earth and the hydrosphere remains an outstanding challenge. Complex system heterogeneity, limited information, and unknown component interaction at all relevant levels may force geologists to turn to advanced stochastic models, such as fractional calculus-based governing equations, whose rigorous development can be best provided by qualified mathematicians. Hence, a close collaboration between geologists and mathematicians is required to develop the next-generation physical models for a broad range of geological dynamics in the hydrosphere and solid Earth. This study provides the first extensive review of major solid Earth dynamics and hydrologic processes that might be addressed by fractional calculus in the next several decades.

In the hydrosphere, non-Fickian dynamics have been well-documented for water flow and chemical transport through heterogeneous aquifers, soils, and rivers consisting of both mobile regions and relatively immobile zones, which can be efficiently quantified by fPDEs that assume random displacement between random waiting times for water (including groundwater, soil moisture, and overland flow), pollutants, and sediment. Future research directions of fractional calculus in the hydrosphere may include the development and application of fPDEs in characterizing real-world-complex hydrologic dynamics that have not been focused on yet, including, for example, complex reactive transport, multiphase and variable density flow, and complex dynamics observed in other aquatic processes.

Future applications of fPDE models in the geological sciences can also focus on solid Earth dynamics, which can be classified into three major groups (i.e., Earth internal processes, large-scale Earth surface processes, and small-scale growth/erosion surface processes), depending on their position and scale. To quantify these three groups of solid Earth dynamics, mechanistic physical models are preferred, and fractional calculus can be added to account for spatial and temporal memories in system dynamics likely missed by traditional models. First, the large-scale, internal Earth dynamics typically involve plastic, viscoelastic, or non-Newtonian advective flow occurring in specific regions with bounded domains. Application of fPDEs in these regions can be challenging due to limited information on the internal Earth, but the lack of fine-scale information is also one of the major reasons to apply fPDEs, which can account for local-scale heterogeneity more efficiently than standard models.

Second, near-surface, large-scale processes with non-Fickian dynamics, which are the most easily recognized and are extensively monitored, include mass movement, landscape evolution, and Aeolian sand dune migration. These processes are controlled by many factors that fluctuate over a wide range of spatial and/or temporal scales. Most Earth surface processes reviewed in this study exhibit alternate random transport (such as materials moving downslope due to gravity, sand dune migration driven by wind, and glacial motion due to gravity and its own weight) and waiting periods (due to, for example, burial of soil particles in soil creep and burial of sand particles in dunes), requiring fPDE models that can distinguish mobile and immobile phases. Considering the abundant data available for surface processes, it is possible that the study of Earth surface dynamics may eventually enhance model predictability by revealing memory kernels.

Third, small-scale growth/erosion surface processes, including crystal growth of minerals, rock/mineral weathering, and pedogenesis, are affected by both physical and chemical factors, and can exhibit similar dynamic behaviors. The KPZ equation, which is the general surface-growth model, can be expanded to account for nonlocal diffusion in both space and time by applying fractional calculus, as already proposed by several studies. The resultant fractional-order KPZ model is expected to capture both random episodicity and nonlocal diffusion-related kinetics in crystal growth under natural geological conditions, and eventually, lead to efficient modeling of transient rock/mineral weathering as well as soil production and transport.

Previous fPDE models have historical challenges in capturing real-world anomalous diffusion, especially those associated with complex solid Earth dynamics. This is similar to the status of other stochastic theories in hydrologic applications. Stochastic subsurface hydrology still cannot capture the nuance of groundwater flow and transport after ∼40 years of research. Future technical development for the fPDE models should at least include predictable spatiotemporal nonlocality, correct mathematical specification of bounded fractional diffusion, efficient characterization of spatiotemporally nonstationary transport, and efficient governing equations for specific kinetics.

Challenge and opportunity exist simultaneously in the application of fractional calculus in Earth system dynamics. Development of fPDEs may eventually allow (1) different dynamics to be modeled with generalized governing equations and (2) reliable characterization of complex kinetics in the Earth system with spatiotemporal boundaries and strong interactions. It is likely that the fPDE, after substantial extension and validation, may become the next-generation, solid Earth dynamic models. The current bottleneck in the application of fractional calculus in hydrologic sciences might not be the end of a promising stochastic approach, but rather be the early stage of a decade-long effort filled with multiple new research and application directions.

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