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Review

Fractional-order differential models for multiscale transport phenomena in materials and energy systems

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Abstract: Transport in heterogeneous and hierarchical materials often exhibits memory, spatial nonlocality, distributed relaxation, and scale-dependent behavior that cannot be adequately represented by classical local constitutive laws. This review critically examines fractional-order differential models as effective continuum descriptions of multiscale heat, mass, charge, and reactive-species transport in materials and energy systems. It first reviews the principal classes of fractional formulations, including time-, space-, time-space-, variable-, distributed-, tempered-, and selectively fractionalized multiphysics models, and examines how operator definitions, kernel structures, domains, initial and boundary conditions, dimensional consistency, and stochastic or coarse-graining interpretations influence their physical meaning. The review then compares analytical, numerical, data-driven, and hybrid solution strategies while evaluating numerical verification, parameter identification, structural and practical identifiability, uncertainty quantification, model discrimination, and experimental validation. Applications in porous and heterogeneous materials, electrochemical systems, thermal transport, subsurface environments, reactive and degrading media, and engineered functional materials are assessed using three cumulative levels of evidence: phenomenological representation, mechanistic support, and predictive transferability. Classical models are retained as reference baselines throughout. The review shows that fractional models can provide compact descriptions of unresolved multiscale complexity; however, anomalous observations alone do not uniquely identify a fractional mechanism. Their scientific use is warranted only when the selected operator is physically and mathematically defensible, parameters are sufficiently identifiable, credible nonfractional alternatives are outperformed, and predictions remain transferable beyond calibration.

Keywords: fractional-order transport models; anomalous diffusion; multiscale transport; memory and nonlocality; parameter identifiability; materials and energy systems

1. Introduction

Transport phenomena underpin virtually every process in materials science and energy engineering. The transport of heat, mass, charge, momentum, and reactive species governs the performance, efficiency, durability, and reliability of systems such as electrochemical energy-storage devices, porous construction materials, polymer membranes, thermal barrier coatings, catalytic reactors, phase-change materials, geological reservoirs, and multifunctional composites. In these systems, transport rarely occurs within homogeneous media or over a single characteristic length or timescale. Instead, it is influenced by structural heterogeneity, pore connectivity, interfacial resistance, trapping and release processes, long-range interactions, and evolving microstructures, giving rise to transport behavior that frequently departs from the predictions of classical continuum theories [1,2].

Classical transport models based on Fick's law, Fourier's law, Darcy's law, and the Nernst-Planck equation have underpinned transport theory for more than a century. Their success depends on assumptions of local constitutive behavior, characteristic transport scales, and Markovian dynamics. In heterogeneous and hierarchical materials, however, these assumptions can become restrictive because the internal structure spans multiple spatial and temporal scales. Experiments across a wide range of systems have reported anomalous diffusion, non-Fickian breakthrough curves, non-exponential relaxation, power-law impedance responses, long-memory effects, and scale-dependent effective transport properties. These observations show that local integer-order differential equations do not always provide an adequate description of transport [3–5].

Fractional-order differential models have become a widely used approach for representing these nonclassical transport phenomena. By extending differentiation and integration to non-integer orders, fractional calculus provides a natural way to account for memory and spatial nonlocality within continuum models. Time-fractional operators are commonly used to describe hereditary effects and distributed relaxation, while space-fractional operators capture nonlocal transport, long-range interactions, and heterogeneous migration pathways. Importantly, fractional transport equations often provide a bridge between stochastic microscopic descriptions and macroscopic continuum models, allowing the influence of unresolved multiscale structures to be represented through a small number of effective constitutive parameters. Consequently, fractional models have been applied extensively to anomalous diffusion, heat transfer, electrochemical transport, porous-media flow, viscoelastic materials, reactive transport, and many other transport processes in complex materials and energy systems [6–9].

Existing reviews have established important foundations for fractional transport modeling, but most concentrate on particular operator families, computational methods, transport mechanisms, or application domains. Reviews have addressed, for example, fractional diffusion and nonlocal operators, continuous-time-random-walk descriptions of anomalous transport, numerical methods for fractional differential equations, and applications in geological, electrochemical, and thermal systems [10–14]. More recent reviews have broadened such a perspective, although issues such as operator justification, parameter identifiability, comparison with nonfractional alternatives, uncertainty, and predictive transferability are still rarely examined together across materials and energy systems [15,16]. The present review addresses the identified gap through an integrated transport-centered assessment linking mathematical formulation and physical mechanism with computation, inverse identification, validation, and cross-domain application evidence.

The present review takes a transport-centered perspective, treating fractional-order models as effective constitutive descriptions of transport in structurally complex media rather than simply as mathematical generalizations. Particular attention is given to connecting fractional operators with physical mechanisms such as continuous-time random walks, trapping and detrapping, broad residence-time distributions, long-range interactions, hierarchical pore networks, and the coarse-graining of heterogeneous media. The review considers the theoretical foundations and main classes of time-, space-, time-space-, variable-, distributed-, tempered-, and heterogeneous-coefficient formulations, as well as selectively fractionalized reaction-transport and multiphysics systems. Analytical, numerical, data-driven, and hybrid solution strategies are considered alongside inverse identification, uncertainty quantification, model discrimination, and experimental validation. Applications are examined across porous and heterogeneous materials, electrochemical systems, thermal transport, subsurface energy systems, reactive and degrading media, and engineered functional materials. Bringing these aspects together allows the review to examine the connections among mathematical formulation, transport mechanisms, physical evidence, and predictive capability, while distinguishing physically supported fractional models from those used primarily as phenomenological descriptions.

The literature considered in the present review was identified through structured searches of Web of Science and Scopus using complementary query groups that covered fractional operators and physical foundations, numerical methods, inverse identification and validation, materials applications, and energy, subsurface, and reactive systems. Relevant reviews and primary studies were then assessed for their contributions to mathematical formulation, physical interpretation, computational verification, parameter identification, comparison with competing models, experimental validation, and predictive performance.

The article is organized as follows. Section 2 introduces the theoretical background of fractional calculus and discusses the mathematical and physical meaning of fractional operators in transport modeling. Section 3 reviews the main classes of fractional transport models and considers the conditions under which their use is scientifically justified. Section 4 examines analytical, numerical, data-driven, and hybrid computational methods, together with parameter identification, uncertainty quantification, model discrimination, and experimental validation. Section 5 focuses on applications in materials and energy systems and discusses the field's main scientific contributions, current limitations, remaining challenges, and possible directions for future research. Section 6 concludes by summarizing the key findings of the review.

2. Theoretical foundations of fractional-order transport modeling

2.1. Fractional calculus as a framework for multiscale transport

Classical transport theory is based on local constitutive laws and integer-order differential equations. Models derived from Fick's law, Fourier's law, Darcy's law, and related formulations have successfully described diffusion, heat conduction, fluid flow, and charge transport in homogeneous media with well-defined spatial and temporal scales. However, their underlying assumptions become increasingly restrictive in materials and energy systems with structural heterogeneity, hierarchical organization, and coupled transport processes. In such systems, transport can be influenced by trapping and release mechanisms, tortuous pathways, long-range interactions, distributed relaxation times, and evolving microstructures. These effects can lead to anomalous diffusion, non-exponential relaxation, and scale-dependent effective properties that are not always adequately captured by classical frameworks [17,18].

Fractional calculus extends conventional differentiation and integration to non-integer orders, offering a continuum framework for transport processes that involve memory and spatial nonlocality. Instead of describing transport as entirely local and instantaneous, fractional formulations account for the influence of past states or interactions over spatial distances within the governing equations. Time-fractional operators are commonly used to describe hereditary behavior arising from broad relaxation spectra and long-memory effects, while space-fractional operators capture transport associated with nonlocal migration pathways or heavy-tailed displacement statistics. Fractional-order models can thus describe multiscale transport without requiring explicit resolution of every underlying microscale process or structural feature [19,20].

Fractional operators are not interchangeable because their definitions determine the form of temporal memory or spatial interaction, the admissible initial and boundary data, the dimensions of generalized transport coefficients, and the corresponding numerical formulation [21,22]. Section 2.2 examines these mathematical differences and their consequences for transport modeling.

A major advantage of fractional transport models is their ability to connect microscopic complexity with macroscopic continuum behavior. Rather than resolving every pore, interface, defect, or stochastic transport event, fractional operators can represent their combined influence through effective constitutive equations. The effective continuum provides a practical middle ground between detailed microscale simulations and conventional continuum models that may miss important multiscale effects. At the same time, reproducing anomalous transport behavior does not prove that a fractional formulation is physically unique. Different stochastic or heterogeneous mechanisms can produce similar anomalous signatures, so the physical interpretation of fractional operators and their connection to measurable material properties remain active areas of research [23,24].

2.2. Principal fractional operators and mathematical formulation

The mathematical and physical meaning of a fractional transport model depends on the operator selected, the domain on which it is defined, and the associated initial and boundary data. Operators of the same order are not necessarily equivalent, especially on bounded domains or when their kernels represent different memory laws [25,26]. For clarity, the main definitions are introduced below for $0 < \alpha < 1$ in time and $0 < \beta \leq 2$ in space, with higher-order extensions following similar constructions.

For an absolutely continuous function f on $[0, T]$, the left-sided Caputo derivative is defined by:

$$ {}^{C}D_{0+}^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\tau)^{-\alpha} f'(\tau) d\tau, \ \ 0 < \alpha < 1 \tag{1} $$

The power-law kernel assigns decreasing but persistent weight to the history of f. Since the derivative acts on f', the Caputo derivative of a constant is zero, and initial conditions can usually be specified using conventional values such as concentration or temperature at $t = 0$ For consistency with the governing equations introduced in Section 3, the abbreviated notation ${}^{C}D_{t}^{\alpha}$ is used hereafter for the Caputo derivative with lower terminal $t = 0$, unless another terminal is explicitly specified.

These properties account for the widespread use of the Caputo derivative in engineering transport models [27, 28]. The corresponding Riemann-Liouville derivative is:

$$ {}^{RL}D_{0+}^{\alpha} f(t) = \frac{d}{dt}\left[\frac{1}{\Gamma(1-\alpha)}\int_{0}^{t}(t-\tau)^{-\alpha} f(\tau)d\tau\right], \;\; 0<\alpha<1 \tag{2} $$

For sufficiently regular functions, the Caputo derivative can be written as the Riemann-Liouville derivative of $f(t) - f(0)$. The two formulations are therefore closely related, but they differ in how they treat initialization and singular behavior near $t = 0$. Riemann-Liouville equations naturally accommodate initial data involving a fractional integral of the solution, while Caputo equations more directly use conventional initial values such as $f(0)$. Conversion between the two formulations is valid only when the initial terms and regularity assumptions are treated consistently.

The Grünwald-Letnikov derivative provides a limiting difference representation:

$$ {}^{GL}D_{0+}^{\alpha} f(t) = \lim_{h\to 0^{+}} h^{-\alpha}\sum_{k=0}^{\lfloor t/\mathrm{h}\rfloor}(-1)^{k}\binom{\alpha}{k} f(t-kh) \tag{3} $$

Under appropriate smoothness, extension, and convergence conditions, this representation is equivalent to the Riemann-Liouville derivative. Its main relevance to transport modeling comes from the direct connection it provides to history-dependent discretization. On finite intervals, however, the lower terminal and the extension of f beyond its prescribed domain influence the operator and must therefore be included explicitly in its definition [29].

Time-fractional derivatives can be represented more generally through a causal kernel:

$$ \mathcal{D}_{\mathcal{K}} f(t) = \int_{0}^{t} K(t-\tau) f^{'}(\tau)d\tau \tag{4} $$

The Caputo derivative is associated with a weakly singular power-law kernel. Caputo-Fabrizio formulations instead use a bounded exponential kernel, while Atangana-Baleanu-Caputo formulations are based on a bounded Mittag-Leffler kernel. Because normalization conventions differ, any timescale introduced into the kernel must be chosen so that its argument remains dimensionless. These operators describe different relaxation behavior, so replacing a singular power-law kernel with a bounded one changes the short-time response, initialization, and asymptotic behavior rather than simply offering another numerical form of the same memory process. Their use should therefore be supported by a physically plausible relaxation spectrum and by mathematical properties such as causality, positivity, invertibility, and recovery of the classical limit [30–32]. Variable-order operators additionally require an explicit statement of whether the order is evaluated at the current time, the historical integration time, or through a non-convolution kernel. Distributed-order operators require an admissible weighting measure over the selected range of orders [33,34].

For spatial transport on $\mathbb{R}^d$, the positive fractional Laplacian is most concisely defined through its Fourier multiplier:

$$\mathcal{F}\left[(-\Delta)^{\beta/2}u\right](\xi) = |\xi|^{\beta}\widehat{u}(\xi), \ \ 0 < \beta \leq 2 \tag{5}$$

For sufficiently regular and decaying functions and $0 < \beta < 2$, the equivalent singular-integral representation is:

$$(-\Delta)^{\beta/2}u(x) = C_{d,\beta}PV\int_{\mathbb{R}^d}\frac{u(x)-u(y)}{|x-y|^{d+\beta}}dy \tag{6}$$

where $C_{d,\beta} > 0$ is a normalization constant and PV denotes the Cauchy principal value. The Riesz fractional derivative is commonly represented, up to sign convention, by $-(-\Delta)^{\beta/2}$. At $\beta = 2$, the fractional Laplacian reduces to the classical negative Laplacian. These definitions describe symmetric whole-space nonlocality; anisotropic or directionally biased transport requires more general Lévy measures or directional fractional operators [35].

On a bounded domain Ω, whole-space definitions that are equivalent on $\mathbb{R}^d$ generally produce different operators. The integral or restricted fractional Laplacian requires values on the exterior $\mathbb{R}^d \setminus \Omega$, rather than data only on the geometric boundary. By contrast, the spectral fractional Laplacian is defined using the eigenpairs $(\lambda_n, \ \phi_n)$ of a specified local Laplacian:

$$(-\Delta_\Omega)^{\beta/2}\,u = \sum_{n=1}^{\infty}\lambda_n^{\beta/2}\,(u,\phi_n)_{L^2(\Omega)}\phi_n \tag{7}$$

Its meaning, therefore, depends on whether the underlying eigenproblem uses Dirichlet, Neumann, Robin, or another boundary condition. Regional, killed, censored, and reflected operators correspond to further distinctions in the treatment of jumps at the domain boundary. These formulations are not interchangeable: operator and boundary-condition selection jointly determine the stochastic process, conservation properties, and solution behavior [36,37].

Fractional operators also change the dimensional structure of transport equations. A time derivative of order α has dimensions $T^{-\alpha}$, while a spatial operator of order β has dimensions $L^{-\beta}$. A generalized coefficient in a time-space fractional diffusion equation consequently has dimensions $L^{\beta}T^{-\alpha}$. Variable- and distributed-order models must either use appropriate reference scales or define coefficients and weighting measures so that dimensional consistency is preserved across orders.

Well-posedness cannot be inferred from the presence of a fractional derivative alone. Existence, uniqueness, regularity, positivity, and conservation depend on the kernel, operator domain, function spaces, data, and boundary conditions. Common linear theories employ causal kernels with suitable positivity or complete-monotonicity properties and nonnegative self-adjoint or sectorial spatial operators. Weak formulations are typically posed in $L^2(\Omega)$ and appropriate fractional Sobolev spaces, such as $H_0^{\beta/2}(\Omega)$ for selected zero-exterior problems. Other operators require different energy spaces. Initial singularities are also common in time-fractional evolution even for smooth data and must be considered in both analysis and numerical approximation [38,39].

Operator selection should therefore be treated as a combined mathematical and constitutive decision. A defensible formulation must specify the derivative definition, kernel, lower terminal, operator domain, initial and boundary data, coefficient dimensions, and classical limit. The operator-definition requirements provide the mathematical basis for connecting the operators to microscopic transport mechanisms in Section 2.3 and for interpreting their physical significance in Section 2.4.

2.3. From microscopic mechanisms to macroscopic fractional equations

A central theoretical justification for fractional transport models is that they can arise as scaling limits of specified stochastic or multiscale processes rather than being introduced solely as mathematical generalizations. The stochastic basis is therefore conditional. A fractional equation emerges only when the underlying probability laws, correlations, and asymptotic limits are consistent with the chosen operator. Stochastic derivations can establish plausible connections between microscopic dynamics and continuum equations, but they do not show that every anomalous transport process must be fractional [40].

The continuous-time random walk (CTRW) framework provides the clearest example. In a Markovian CTRW with exponentially distributed waiting times and finite-variance displacements, appropriate scaling generally leads to a classical advection-diffusion equation. If the waiting-time distribution instead has a persistent heavy tail while the jump variance remains finite, the scaling limit can produce a time-fractional equation that describes subdiffusive transport. When the jump distribution belongs to the domain of attraction of a symmetric stable law, the continuum limit can involve a Riesz derivative or fractional Laplacian; asymmetric stable limits lead to directional or skewed spatial operators. If heavy-tailed waiting times and displacements are statistically independent, a separable time-space fractional equation may emerge. Direct dependence between displacement length and travel duration, as occurs in coupled CTRWs or finite-velocity Lévy walks, can instead produce fractional material derivatives or other nonseparable operators. The resulting fractional structure therefore depends on the specific statistics of the underlying process, not simply on the presence of heavy tails [19,23,41–43].

Generalized master equations offer a complementary route for deriving fractional transport models. In these formulations, the transition dynamics include explicit temporal memory kernels or spatially nonlocal transition measures. Under appropriate limiting conditions, power-law kernels can give rise to fractional evolution operators, while truncated, tempered, or multiscale kernels lead to different constitutive forms. From this perspective, the fractional derivative represents the macroscopic effect of a particular memory law rather than an independently introduced modification of classical transport [44,45].

Homogenization, model reduction, and coarse-graining provide another, related route. Transport may still follow local classical laws at the microscale, while eliminating unresolved variables at larger scales introduces memory, nonlocal fluxes, or history-dependent effective coefficients. Features such as pores, fractures, grain boundaries, particle networks, and interfaces can generate broad residence-time distributions or persistent spatial correlations when viewed over experimentally accessible scales. Fractional operators may then serve as effective closures, but their emergence depends on the underlying statistical structure; heterogeneity by itself does not guarantee a fractional macroscopic limit [46,47].

The coarse-graining perspective is especially relevant to materials and energy systems where resolving every transport pathway directly is impractical. In porous electrodes, for example, ionic transport is shaped by tortuous pores, particle connectivity, interfacial transfer, and changes in microstructure. In fractured geological media, fracture-matrix exchange and broad residence-time distributions can produce long temporal tails and nonlocal spreading. Similar arguments can be made for heterogeneous thermal and composite materials. These examples show how fractional behavior may emerge from unresolved structure, but they do not identify a unique operator unless the underlying statistics are independently characterized [48–50].

The link between microstructure and operator choice remains one of the least developed areas of fractional transport modeling. In many engineering applications, a fractional equation is proposed and its parameters are estimated from macroscopic observations rather than derived from independently measured waiting-time, displacement, connectivity, or relaxation statistics. As a result, different microscopic mechanisms can lead to similar effective fractional orders, while the same material may require different operators at different scales or under different operating conditions. Progress toward predictive modeling, therefore, depends on establishing relationships between measurable microstructural descriptors and the operator type, fractional order, kernel, and generalized transport coefficients, followed by validation against observations that were not used for calibration [51,52].

2.4. Physical interpretation and limitations of fractional transport models

Within a given model, temporal and spatial fractional operators represent different constitutive assumptions. A time-fractional derivative accounts for the influence of previous states through a chosen kernel and may be associated with trapping, delayed release, or distributed relaxation. A space-fractional operator describes interactions or displacements beyond an immediate neighborhood and may represent preferential pathways or long-range connectivity. These interpretations are physically meaningful only when the chosen kernel or spatial measure is consistent with the underlying mechanisms and the observational scale of the system [53,54].

Macroscopic anomalous behavior does not point uniquely to a fractional mechanism. Non-Fickian breakthrough curves, non-exponential relaxation, and heavy-tailed responses can also result from multirate mass transfer, mobile-immobile transport, distributed reaction kinetics, spatially heterogeneous classical coefficients, evolving material properties, or measurement and coarse-graining effects. As a result, different models may reproduce the same observable with similar accuracy while implying different underlying physics. Fractional formulations are therefore best treated as effective constitutive hypotheses that should be evaluated against plausible competing descriptions [55–57].

The fractional order should be interpreted with the same degree of caution. In a specified time-fractional model, a lower order is often associated with stronger memory and slower relaxation, while in a specified space-fractional model, the order governs the scaling and tail behavior of the corresponding nonlocal process. Even so, a fitted fractional order should not be treated as a universal material constant. Its value can depend on the operator definition, measurement interval, specimen size, boundary conditions, operating state, and coupling with other processes. Different microscopic mechanisms may produce similar effective orders, and the same material may exhibit different values across scales or experimental conditions [58,59].

The main theoretical challenge is not simply whether a fractional equation can fit anomalous data, but whether the chosen operator is identifiable, mathematically admissible, and preferable to competing models. A defensible interpretation requires agreement among the observed transport behavior, microscopic or microstructural evidence, kernel or jump statistics, initial and boundary conditions, and the dimensional structure of the governing equation. Properties such as positivity, conservation, stability, and thermodynamic compatibility must be demonstrated for the complete model rather than assumed from the fractional operator alone [60, 61]. Mechanistic claims, therefore, require evidence beyond calibration, while models supported only by curve fitting should be described clearly as phenomenological or reduced-order representations.

Fractional transport models therefore occupy a middle ground between resolved microscopic descriptions and classical local continuum equations. They can retain important effects of unresolved structure while remaining suitable for continuum analysis and computation, although their predictive value depends on parameter identifiability and validation beyond the conditions used for calibration. Section 3 examines how these theoretical principles are incorporated into the main families of fractional governing equations. Section 4 then considers their analytical and numerical solution, parameter identification, uncertainty quantification, model discrimination, and experimental validation.

3. Fractional differential models for multiscale transport phenomena

3.1. Fractional transport equations: From anomalous observations to governing models

Fractional transport equations have emerged to describe transport behaviors that are not always captured adequately by classical continuum models. Across porous media, electrochemical devices, polymers, composites, and geological formations, experiments have revealed subdiffusion and superdiffusion, non-Fickian breakthrough curves, power-law relaxation, non-Gaussian spreading, and scale-dependent transport properties. These signatures are commonly associated with interactions among heterogeneous microstructures, broad temporal and spatial scales, trapping processes, and long-range connectivity. They do not, however, uniquely establish fractional dynamics, because related behavior may also arise from heterogeneous but local transport, multirate exchange, distributed kinetics, or evolving material properties [62–65].

Classical equations based on Fick, Fourier, Darcy, and Nernst-Planck formulations remain appropriate when transport can be described through local constitutive relations and well-defined characteristic scales. When adjustments to local coefficients are insufficient, fractional differential equations provide one possible generalization of the constitutive structure. Temporal operators introduce memory into the evolution law, whereas spatial operators represent nonlocal migration. As discussed in Section 2, these formulations can be connected to continuous-time random walks, generalized master equations, and multiscale coarse-graining, but their use in a particular system still requires evidence that the selected operator represents the dominant transport mechanism [66–68]. Throughout Section 3, $c(x,t)$ denotes the transported field, $x \in \Omega \subset R^d$ denotes spatial position, and α and β denote the temporal and spatial fractional orders, respectively.

Different anomalous signatures have consequently motivated distinct model families. Time-fractional equations primarily address memory and distributed relaxation, whereas space-fractional equations represent nonlocal migration and heavy-tailed spatial statistics. Coupled time-space formulations combine both effects when temporal and spatial evidence support their simultaneous inclusion. Generalized models introduce variable or distributed orders, heterogeneous coefficients, or state-dependent constitutive structure to describe evolving media. Fractional operators may also be incorporated selectively into reaction-transport and multiphysics systems in which anomalous transport interacts with chemical, thermal, electrical, or mechanical processes [69–72].

The choice among these formulations is a constitutive modeling decision rather than a purely mathematical one. It should account for the observed anomaly, mechanistic and microstructural evidence, parameter identifiability, boundary and interface conditions, computational tractability, and predictive performance relative to classical and non-fractional alternatives. Sections 3.2–3.6 examine the principal model families, while Section 3.7 develops an explicit framework for their comparative assessment and selection. Together, these discussions establish the governing-model basis for the numerical, inverse, and validation methods considered in Section 4.

3.2. Time-fractional transport models

Time-fractional models describe transport in which the present evolution depends on the prior history of the system. To state the mathematical specification explicitly, consider a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ and a finite observation interval $0 < t \leq T$. A canonical initial-boundary-value problem is:

$$\begin{cases} {}^{C}D_t^{\alpha} c(x,t) = \nabla \cdot [D_\alpha \nabla c(x,t)] + s(x,t), & x \in \Omega, 0 < t \leq T, 0 < \alpha < 1, \\ c(x,0) = c_0(x), & x \in \Omega, \qquad 0 < \alpha < 1, \\ c(x,t) = 0, & x \in \partial\Omega, \qquad 0 < t \leq T, \end{cases} \tag{8}$$

here, ${}^{C}D_0^{\alpha}$ denotes the Caputo derivative with lower terminal $t = 0$, defined by:

$$ {}^{C}D_t^{\alpha} c(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\tau)^{-\alpha} \frac{\partial c(x,\tau)}{\partial \tau} \, \mathrm{d}\tau. \tag{9} $$

The generalized diffusivity $D_\alpha > 0$ has dimensions:

$$ [D_\alpha] = L^2 T^{-\alpha}, \tag{10} $$

whereas the source term must satisfy:

$$ [s] = [c] T^{-\alpha}. \tag{11} $$

The homogeneous Dirichlet condition is used here to provide a complete illustrative formulation. Neumann, Robin, mixed, or interface conditions define different mathematical problems and must be stated explicitly. For:

$$ c_0 \in L^2(\Omega), \;\; s \in L^2 \left(0, T; L^2(\Omega)\right), \;\; D_\alpha > 0 \tag{12} $$

For the stated linear problem, standard linear theory provides a unique weak solution in the energy setting associated with $H_0^1(\Omega)$, subject to the regularity and compatibility assumptions of the selected formulation. Time-fractional solutions may nevertheless exhibit reduced regularity near $t = 0$, even when the prescribed data are smooth, and the reduced initial-time regularity behavior must be considered in numerical approximation [73, 74].

In the integer-order limit,

$$ \alpha \to 1, \;\; {}^{C}D_t^{\alpha} c \to \frac{\partial c}{\partial t}, \;\; D_\alpha \to D_1 \tag{13} $$

and the problem reduces to the conventional diffusion equation:

$$ \frac{\partial c(x,t)}{\partial t} = \nabla \cdot [D_1 \nabla c(x,t)] + s(x,t) \tag{14} $$

with the same initial and boundary data. For the homogeneous unbounded problem, the time-fractional formulation produces subdiffusive scaling and non-exponential temporal relaxation.

The physical basis of the time-fractional formulation is commonly associated with broad waiting-time or relaxation distributions. In porous, polymeric, electrochemical, and geological media, transported species may undergo repeated immobilization, delayed release, or migration through regions with widely differing local mobilities. These mechanisms generate long-lived temporal correlations that cannot always be represented by a single relaxation time. The fractional derivative replaces that assumption with a memory kernel, providing a compact constitutive representation of unresolved temporal heterogeneity [75–77].

Time-fractional formulations have been extended to advection-diffusion, heat-transfer, electrochemical, and reaction-transport problems. Their appropriate use depends on identifying which part of the governing model possesses memory.

A fractional accumulation term, a memory-dependent flux closure, and a fractional kinetic relation represent distinct constitutive assumptions and should not be treated as interchangeable [78, 79]. Reaction-transport coupling requires particular care because reaction processes can interact directly with the underlying waiting-time dynamics. CTRW-based derivations show that simply replacing the classical diffusion term with a fractional counterpart does not, in general, produce the correct reaction-subdiffusion equation [80, 81].

The interpretation of the fractional order must remain conditional. Constant-order models usually imply power-law memory over the modeled interval, whereas many materials exhibit crossover behavior as their structure, state, or operating conditions change. Non-exponential transients may also arise from multirate exchange, distributed reaction kinetics, heterogeneous classical coefficients, or measurement filtering [82,83]. A time-fractional model is therefore most convincing when temporal data support a persistent memory law, the inferred parameters are identifiable, and predictions remain valid outside the calibration interval. When anomalous behavior is controlled primarily by spatial connectivity rather than temporal retention, a space-fractional formulation may provide a more appropriate constitutive description.

3.3. Space-fractional transport models

Space-fractional transport models describe systems in which migration cannot be represented adequately through local spatial gradients or nearest-neighbor interactions. A canonical isotropic space-fractional diffusion equation on an unbounded domain can be written as:

$$\frac{\partial c(x,t)}{\partial t} = -K_\beta(-\Delta)^{\beta/2}c(x,t) + s(x,t), \;\; 1 < \beta \leq 2 \tag{15}$$

where $(-\Delta)^{\beta/2}$ is the fractional Laplacian, K_β is a generalized transport coefficient with dimensions that depend on β, and s is a source term. For the isotropic operator on an unbounded domain, the fractional Laplacian is associated with the Fourier multiplier $|k|^\beta$. The classical diffusion equation is recovered when $\beta = 2$. On the whole space, space-fractional diffusion and related fractional Fokker-Planck equations are closely connected to Lévy-stable stochastic processes and heavy-tailed displacement statistics [84, 85].

The stochastic basis of space-fractional transport is commonly associated with heavy-tailed jump-length distributions and Lévy-type transport. In physical materials, however, the operator should not necessarily be interpreted as a carrier making arbitrarily long instantaneous jumps. It may instead represent the effective macroscopic consequences of preferential channels, network shortcuts, fracture connectivity, or other unresolved pathways that produce apparently nonlocal transport at the observation scale. Truncation of the underlying heavy tails can also produce a crossover from superdiffusive to approximately classical behavior, emphasizing that a pure Lévy-stable model need not remain appropriate over all scales [86, 87]. The distinction between literal long jumps and an effective description of nonlocal transport is therefore important when a fitted spatial order is interpreted in relation to the material's actual architecture.

Space-fractional formulations have been used extensively to describe non-Gaussian plume evolution and unusually rapid spreading in heterogeneous and fractured porous media. They have also been applied to nonlocal heat and species transport in disordered porous materials. Their main advantage is that heavy-tailed or asymmetric spatial distributions can be represented without explicitly resolving every preferential pathway [88–90]. The physical interpretation is most convincing when spatially resolved measurements or structural characterization independently support long-range connectivity, broad velocity distributions, or heavy-tailed displacement statistics.

Finite domains introduce an additional complication because integral, spectral, regional, killed-process, censored, and reflected forms of fractional spatial operators generally describe different nonlocal interactions and boundary behavior. The choice among these formulations determines how trajectories interact with the exterior of the domain, including whether they are absorbed, censored, reflected, or otherwise constrained. Conventional Dirichlet, Neumann, or Robin terminology is therefore not sufficient unless the operator and its associated exterior or boundary prescription are defined explicitly [91, 92]. The operator-boundary distinction is particularly important for confined systems such as membranes, thin films, separators, and finite electrochemical devices.

Non-Gaussian spreading does not by itself establish spatially fractional transport. Similar behavior can arise from spatially heterogeneous but local diffusivities, correlated velocity fields, unresolved advection, network transport, or mixtures of classical pathways [93–95]. A space-fractional model is therefore most defensible when it improves prediction beyond these alternatives and when its operator, boundary treatment, and inferred order are consistent with the physical transport mechanism. When independent evidence also indicates persistent temporal memory, a coupled time-space formulation may be required, as considered in the following subsection.

3.4. Time-space fractional transport models

Many complex transport systems exhibit temporal memory and spatial nonlocality concurrently. Time-space fractional models represent these effects within a single governing equation by combining the temporal and spatial operators introduced in Sections 3.2 and 3.3. A canonical time-space fractional diffusion equation can be written as:

$$ {}^{C}D_t^{\alpha} c(x,t) = -K_{\alpha,\beta}(-\Delta)^{\beta/2} c(x,t) + s(x,t), \ \ 0 < \alpha \leq 1, \ 1 < \beta \leq 2 \tag{16} $$

where α characterizes temporal memory, β controls the degree of spatial nonlocality, $K_{\alpha,\beta}$ is a generalized transport coefficient with dimensions $L^{\beta}T^{-\alpha}$, and $s(x,t)$ denotes a source or sink. The classical diffusion equation is recovered when $\alpha = 1$ and $\beta = 2$, whereas the limiting cases $\beta = 2$ and $\alpha = 1$ recover the time- and space-fractional formulations, respectively [96,97].

An important distinction concerns the meaning of time-space coupling. The equation above contains fractional operators in both variables, but its simplest stochastic interpretation generally treats the waiting-time and jump-length statistics as separable. The time-space fractional formulation therefore combines temporal memory and spatial nonlocality without necessarily representing a direct statistical dependence between them. If displacement length is explicitly linked to travel duration, as in finite-velocity Lévy walks or other coupled continuous-time random walks, the appropriate continuum description may instead require a nonseparable memory kernel, a fractional material or substantial derivative, or another operator that preserves the underlying space-time dependence [42, 98, 99]. The distinction between separable and genuinely coupled space-time dynamics is essential because inserting separate time- and space-fractional derivatives into the same equation does not automatically reproduce the physics of a genuinely coupled stochastic process.

Time-space formulations are most useful when observations provide evidence for both persistent temporal tails and non-Gaussian or anomalously broad spatial transport. Experimental and application studies have used such formulations in strongly heterogeneous porous media where retention processes coexist with preferential or nonlocal migration. Chang and Sun, for example, applied time-space fractional derivative models to CO_2 transport in heterogeneous media and compared the simulations with experimental breakthrough data, while Kang et al. validated a model containing both temporal and spatial fractional derivatives against gas adsorption-desorption experiments in heterogeneous coal [100, 101]. In these settings, a time-fractional model may reproduce delayed breakthrough while failing to describe spatial spreading, whereas a space-fractional model may represent nonlocal migration without capturing long-time retention. Incorporating both operators can therefore improve the simultaneous description of temporal and spatial observables.

The additional flexibility also creates a substantial identifiability problem. In the simplest unbounded models, the characteristic spreading scale depends on a combination of the fractional orders, typically through α/β. Measurements of plume width or bulk spreading alone may therefore constrain only this combination rather than identifying α and β separately. Correlation with the generalized transport coefficient can further produce several parameter combinations with similar predictive errors. Reliable calibration, therefore, requires measurements that capture both temporal and spatial behavior, such as time-dependent concentration fields, breakthrough curves recorded at multiple locations, or complementary information on residence-time and displacement statistics [102, 103]. Boundary treatment must also remain consistent with the chosen spatial operator, as discussed in Section 3.3.

Time-space fractional models are therefore warranted when single-operator formulations cannot reproduce independently observed temporal and spatial signatures and when both mechanisms have plausible physical support. Their performance should be compared with alternatives such as multirate mass-transfer models, mobile-immobile formulations, and heterogeneous classical transport equations before the additional fractional order is accepted. Comparison with multirate and heterogeneous classical alternatives can materially change the interpretation: for example, multirate descriptions have reproduced transport behavior that might otherwise be attributed to fractional memory, and experimental coal-gas data have been interpreted successfully using a distribution of classical diffusion rates rather than a fractional time derivative [104, 105]. When the inferred memory or nonlocality changes with position, time, material state, or operating conditions, constant-order time-space equations may remain insufficient; such behavior motivates the generalized fractional models considered next.

3.5. Generalized fractional transport models

Constant-order fractional equations assume that the form and strength of anomalous transport remain unchanged throughout the domain and observation period. The constant-order approximation may become inadequate when material structure, operating conditions, or dominant transport mechanisms change over time or space. Variable-order, distributed-order, and heterogeneous-coefficient formulations extend the models introduced in Sections 3.2–3.4 by allowing memory, nonlocality, or transport intensity to vary within the constitutive description. Because these formulations represent different physical situations, they should not be treated simply as interchangeable ways of increasing model flexibility [9, 58].

In a variable-order model, the fractional order varies with position, time, or system state. In nondimensional variables, an illustrative time-fractional formulation is:

$$
\begin{gathered}
{}^{C}D_t^{\alpha(x,t)} c(x,t) = \nabla \cdot [D(x,t,c)\nabla c(x,t)] + s(x,t), \\
0 < \alpha_{min} \le \alpha(x,t) \le \alpha_{max} \le 1
\end{gathered} \tag{17}
$$

Here, changes in the fractional order represent changes in the effective memory law, while changes in the transport coefficient reflect variations in transport intensity. The distinction matters because a coefficient that varies in space or time does not necessarily indicate a change in the degree of anomalous transport. Variable-order formulations are most convincing when independent observations point to a transition between transport regimes, for example, during microstructural degradation, phase transformation, pore evolution, or changes in saturation or temperature. Without such evidence, a fitted order function may simply absorb variations that could be described more transparently using conventional state-dependent coefficients [59, 106, 107].

The mathematical definition of a variable-order derivative must also be specified clearly. Several nonequivalent formulations are possible, depending on whether the order is evaluated at the current time, at the historical integration time, or through a more general kernel. Because these formulations assign different weights to past states, they represent different physical memory laws. Specifying only $\alpha(t)$without defining how it enters the memory kernel is therefore not enough to determine the governing equation uniquely [33, 69, 108].

Distributed-order models provide a different type of generalization. Rather than assigning a single order at each point, they combine a range of fractional orders through a weighting function:

$$
\mathcal{D}_t^{(\mu)} c(x,t) = \int_{\alpha_{\min}}^{\alpha_{\max}} \mu(\alpha)\, {}^{C}D_t^{\alpha} c(x,t)\, \mathrm{d}\alpha. \tag{18}
$$

The weighting function $\mu(\alpha)$ specifies how strongly different memory exponents contribute to the overall response. Distributed-order formulations can therefore represent broad or overlapping relaxation spectra, ultraslow transport, and transitions that are not captured by a single power-law kernel. Their physical meaning, however, depends on whether the weighting distribution can be related to measurable relaxation processes or distinct transport populations. The admissibility, units, support, and regularity of $\mu(\alpha)$ must also be specified; otherwise, the distributed-order operator risks becoming an unconstrained fitting device [34, 70, 109].

Tempered and truncated fractional models offer another extension when power-law memory or displacement statistics hold only over a limited range. By introducing a cutoff into the temporal memory kernel or spatial jump distribution, these formulations allow transport to move gradually toward classical behavior at sufficiently long times or large distances and can also recover finite statistical moments. The cutoff, however, introduces an additional characteristic scale that must be identified independently of the fractional order and transport coefficient [45, 72, 87].

Variable coefficients and heterogeneous domains offer another way to generalize the constitutive description. The coefficients may vary with position, time, concentration, temperature, porosity, damage, or other state variables, while the fractional orders remain fixed. In nonlocal equations, the placement of a coefficient is part of the model definition because multiplication by a heterogeneous coefficient generally does not commute with fractional spatial differentiation. A coefficient placed outside a fractional operator, included within a nonlocal flux, or applied through a coefficient-weighted field can therefore lead to physically and mathematically different models. Piecewise coefficients or fractional orders also require suitable interface conditions to maintain flux continuity, conservation, and consistency across adjacent material regions [110, 111].

The main limitation of these generalized formulations is parameter identifiability. Changes in fractional order, transport coefficient, source behavior, or boundary conditions can produce similar observable responses. Adding more constitutive functions may therefore improve calibration while making the model less unique and less reliable outside the calibration range. Recent inverse studies show that spatially varying or distributed fractional orders can be recovered only under specific assumptions about the observations, solution regularity, and medium properties, which reinforces the need to distinguish true mathematical identifiability from flexible curve fitting [112, 113]. Generalized models should therefore be used only when constant-order alternatives show systematic and physically interpretable shortcomings, and when the available data can separately constrain the proposed spatial, temporal, or state dependence. Regularization, uncertainty analysis, and comparison with simpler heterogeneous classical models are essential for determining whether the additional constitutive freedom is warranted.

Variable-order, distributed-order, tempered, and heterogeneous-coefficient models thus provide useful descriptions of evolving or structurally nonuniform transport, but their flexibility must be constrained by physical evidence and mathematical admissibility. When transport evolution is additionally coupled to reactions, heat transfer, electrochemical fields, deformation, or other physical processes, these generalized constitutive laws become components of the multiphysics frameworks considered in the following subsection.

3.6. Fractional reaction-transport and multiphysics models

Transport in materials and energy systems is frequently coupled to chemical reactions, heat transfer, electric fields, mechanical deformation, or microstructural evolution. Fractional reaction–transport and multiphysics models extend the preceding formulations by coupling anomalous transport with one or more of these processes. Unlike the canonical single-field models considered in Sections 3.2–3.5, however, no single governing form is generally applicable because the placement of fractional operators depends on the microscopic reaction mechanism and on which constitutive processes exhibit memory or spatial nonlocality [80,81,114].

The placement of the reaction term requires particular care. In a Markovian reaction-diffusion equation, transport and reaction contributions can often be added independently. The additive separation of reaction and transport does not generally remain valid when transport contains memory. If the reaction proceeds while particles are trapped, the reaction survival probability modifies the waiting-time statistics and, consequently, the memory kernel governing transport. A reaction occurring only during mobile periods produces a different macroscopic equation. Depending on the microscopic mechanism, the memory operator may act on transport alone, on a combination of transport and reaction terms, or through a reaction-dependent substantial derivative. These formulations are not mathematically equivalent, even when they contain the same fractional order and reaction-rate constant. Simply adding a conventional reaction term to a fractional diffusion equation does not, by itself, produce a physically consistent reaction-subdiffusion model [114–116].

Dimensional consistency alone is also not enough to justify a particular coupling law. For example, multiplying a conventional reaction rate, with units of concentration per unit time, by a characteristic-time factor can make it dimensionally compatible with a time-fractional equation. However, that rescaling does not show that the resulting formulation follows from the underlying reaction and transport mechanisms. Where possible, the operator structure should instead be derived from particle-level kinetics, generalized master equations, or clearly stated constitutive assumptions [117–119].

The same principle applies to multiphysics formulations. Fractional operators have been used in models of electrochemical transport, thermo-diffusion, reactive porous media, and damage-coupled mechanics [120, 121]. However, replacing every temporal or spatial derivative in a coupled model with a fractional operator is rarely necessary or physically justified. A more defensible approach is selective fractionalization, in which fractional operators are introduced only into those balance equations for which experiments or microscale arguments support memory or spatial nonlocality, while the remaining fields retain classical governing equations. For example, anomalous ionic transport may occur alongside classical charge conservation, while memory-dependent mass transport may be coupled to a conventional mechanical equilibrium equation.

The resulting system must still satisfy the relevant conservation laws, interface conditions, and constitutive constraints. Mass and charge sources need to remain balanced across the coupled equations, while nonlocal spatial fluxes require boundary prescriptions that are consistent with the chosen fractional operator. Constitutive terms should also be checked for positivity, dissipation, and thermodynamic admissibility. These requirements become especially important when fractional parameters depend on temperature, concentration, damage, or other evolving state variables, because unconstrained coupling functions can yield nonphysical solutions even when the model fits the calibration data well [61, 122].

Coupled models also pose substantial challenges for parameter identification and validation. Changes in fractional order, reaction kinetics, transport coefficients, and coupling strengths can produce similar transient responses, making it difficult to separate their individual effects. Calibration against a single observable, such as concentration or voltage, may therefore be inadequate. More reliable identification requires simultaneous measurements of multiple fields, targeted perturbation experiments, uncertainty analysis, and validation under conditions that were not used for calibration. The additional complexity is justified only when a fractional multiphysics model improves the joint prediction of coupled observables and offers a clear advantage over simpler classical or single-physics alternatives.

Fractional reaction-transport and multiphysics formulations can therefore provide useful reduced-order descriptions of interacting processes across multiple scales. Their scientific value depends less on how many fractional operators are included and more on whether the placement, dimensional structure, and physical interpretation of each operator are well justified. These issues provide the basis for the comparative model-selection framework developed in the following subsection.

3.7. Comparative assessment and model selection

The fractional formulations reviewed in this section should not be viewed as a hierarchy in which greater mathematical complexity automatically leads to a better transport model. Time-fractional, space-fractional, time-space, generalized, and multiphysics formulations represent different constitutive hypotheses for the origin of anomalous behavior. Model selection should therefore start from the observed transport signatures and the physical mechanisms that could plausibly produce them, rather than from a preferred fractional operator. The classical integer-order model should remain the reference description and should be retained whenever it provides accurate, physically consistent, and transferable predictions [123].

Time-fractional models are most appropriate when the observed anomaly is primarily temporal and can reasonably be linked to trapping, broad residence-time distributions, hereditary effects, or distributed relaxation. Support for such a model should go beyond an improved fit to a single transient curve and may include persistent temporal tails, aging, rate-dependent relaxation, or independent evidence of retention processes. Space-fractional formulations are more appropriate when measurements indicate long-range spatial correlations, preferential pathways, or displacement statistics that cannot be explained by local diffusion with physically reasonable heterogeneous coefficients. Time-space fractional models require evidence that both temporal memory and spatial nonlocality contribute independently, making them difficult to justify when only one type of measurement is used [57, 124].

Generalized formulations require a higher level of supporting evidence. Variable-order models are justified when the effective anomalous regime changes systematically with time, position, material state, or operating conditions. Distributed-order models are more appropriate when observations indicate a spectrum of overlapping memory processes rather than a single fractional exponent. Variable coefficients should be considered separately, since a change in transport intensity is not equivalent to a change in the order of the governing operator. Fractional reaction-transport and multiphysics models should likewise be used when reactions or coupled fields can be shown to alter the underlying memory or nonlocal transport mechanism, rather than simply because several physical processes are present in the same system.

Fractional models should be compared with non-fractional alternatives that can produce similar macroscopic behavior, including heterogeneous classical transport equations, multirate mass-transfer and mobile-immobile models, distributed reaction or relaxation models, delayed constitutive laws, and correlated stochastic processes. Within the fractional family, tempered or truncated formulations should be considered when anomalous scaling occurs only over a finite range. Since several competing models can reproduce heavy-tailed transients or non-Gaussian profiles, goodness of fit alone cannot determine the governing mechanism. Competing formulations should instead be assessed using physically discriminating observables, parameter parsimony, uncertainty, and predictive performance beyond the calibration dataset [125–127].

Identifiability is another important criterion for model selection. A model should not include more independent orders, coefficients, or coupling functions than the available measurements can constrain reliably. Strong correlations between fractional order and transport coefficient, or between temporal and spatial orders, can lead to calibrations that appear accurate but are not unique. Profile likelihoods, posterior distributions, sensitivity analysis, and repeated calibration under different initial and boundary conditions can help reveal such ambiguity. If the parameters are to be interpreted as transferable constitutive descriptors, they should also remain reasonably stable across changes in experimental duration, specimen geometry, concentration range, and operating conditions. Systematic parameter drift may instead point to model-form error, regime dependence, or an inadequately resolved physical mechanism [128, 129].

For the present review, the evidence is assessed at three cumulative levels. Phenomenological representation asks whether the model reproduces the measured anomalous response. Mechanistic support considers whether the selected operator and parameters agree with independent evidence from microstructure, waiting-time statistics, connectivity, relaxation spectra, or other physical observations. Predictive transferability asks whether the model can predict behavior under conditions that were not used for calibration. A fractional model may still be useful as a phenomenological reduced-order description when mechanistic support is incomplete, but the strength of its claims should reflect that limitation. Predictive or constitutive interpretations require support at all three levels.

A defensible model-selection workflow can therefore be organized into six stages: characterize the anomaly using temporal and spatial measurements; identify plausible physical mechanisms; establish classical and generalized non-fractional baselines; select the simplest fractional operator supported by the evidence; assess identifiability, uncertainty, conservation, and mathematical admissibility; and carry out out-of-sample and cross-condition validation. A fractional formulation is scientifically justified when it offers a reproducible predictive advantage, its parameters can be identified with sufficient confidence, and its operator structure is consistent with the proposed transport mechanism. If these conditions are not met, the simpler competing model should be preferred.

The focus, therefore, shifts from showing that fractional equations can fit anomalous data to determining when they provide a justified and predictive constitutive description. Applying these criteria requires reliable analytical and numerical solvers, robust parameter-identification procedures, uncertainty analysis, and appropriate experimental validation. Section 4 focuses on these methodological requirements.

4. Numerical methods, parameter identification, and model validation

4.1. Computational challenges in fractional transport modeling

The nonlocal structure of fractional operators produces computational requirements that differ fundamentally from those of classical local transport equations. A direct discretization of a time-fractional derivative generally requires contributions from all preceding time levels, causing storage and computational costs to increase throughout a transient simulation. Space-fractional operators couple each spatial location to an extended region or, in some formulations, to the entire computational domain. Their discretization therefore often produces dense or globally coupled algebraic systems instead of the sparse matrices associated with local differential operators [130, 131]. These difficulties become more pronounced in multidimensional, nonlinear, variable-order, and multiphysics models.

Numerical implementation is also inseparable from operator definition. Approximating a memory kernel, truncating its history, or compressing its representation may change the long-time response of a time-fractional model. Similarly, the discretization of a space-fractional operator must remain consistent with its domain, exterior or boundary data, and stochastic interpretation, as discussed in Section 2.2. Methods developed for spectral, integral, directional, or regional operators are not automatically interchangeable [132–134]. An algorithm may therefore converge to a mathematically well-defined solution while still representing a different constitutive model from the one originally intended.

Computational methods for fractional transport must consequently be evaluated using criteria beyond execution time and conventional discretization error. The main requirements include consistency with the selected operator, stability, convergence for solutions with limited regularity, conservation and positivity where physically necessary, preservation of asymptotic memory or spreading behavior, and scalability across experimentally relevant spatial and temporal ranges. Time-fractional diffusion solutions, in particular, often exhibit weak singularities near the initial time. As a result, error estimates based on conventional smoothness assumptions can overstate the observed convergence order unless the discretization, mesh grading, or starting corrections account for the reduced regularity [135, 136]. Numerical error must also be distinguished from parameter and model-form uncertainty so that computational artifacts are not mistaken for evidence of anomalous transport. Analytical and semi-analytical solutions provide useful benchmarks for verifying these requirements and are considered in the following subsection.

4.2. Analytical and semi-analytical solution strategies

Analytical and semi-analytical solutions help reveal the scaling behavior, asymptotic limits, and parameter dependence of fractional transport models while providing benchmark cases for computational verification. For linear constant-coefficient problems, Laplace transformation is particularly effective for handling temporal fractional derivatives, whereas Fourier transformation diagonalizes translation-invariant spatial operators on unbounded domains. Combined Laplace-Fourier approaches can therefore reduce time-, space-, and time-space fractional equations to algebraic relations in transform space. The resulting inverse transforms often involve Mittag-Leffler, Wright, or related special functions, whose behavior replaces the exponential relaxation and Gaussian spreading patterns characteristic of classical transport [137, 138].

Green's functions and fundamental solutions describe the response to localized initial data or forcing and are useful for examining positivity, normalization, spreading rates, and long-time asymptotic behavior. On bounded domains, eigenfunction expansions and spectral decompositions provide corresponding solution representations when the spatial operator and boundary conditions admit a suitable basis [139, 140]. These representations depend on the operator chosen, so an expansion based on the spectral fractional Laplacian does not automatically apply to an integral or restricted fractional Laplacian on the same domain [141]. Semi-analytical methods can also combine analytical temporal representations with numerically computed eigenpairs, quadrature, or inverse transforms, extending benchmark solutions to geometries for which fully closed-form expressions are not available.

Similarity analysis and scaling arguments provide further insight into self-similar propagation, anomalous spreading exponents, and transitions between transport regimes [54]. Asymptotic approximations are especially useful when exact inversion of transformed solutions is impractical or when the main interest is in short- or long-time behavior. However, their validity depends on the assumed regularity, coefficient structure, geometry, and initial and boundary data. Numerical inversion of transforms and the evaluation of special functions can also introduce errors and should not be regarded as exact simply because the underlying representation is analytical [142].

The main value of analytical and semi-analytical methods is both interpretive and computational. They help isolate the effects of fractional order and operator choice under controlled conditions, support consistency and convergence testing, and provide synthetic data for evaluating inverse algorithms. Their use becomes more limited for nonlinear, heterogeneous, variable-order, and strongly coupled systems, where direct discretization is generally required. The numerical treatment of time-fractional operators is considered next.

4.3. Discretization of time-fractional operators

Time-fractional derivatives are commonly approximated using convolution formulas that preserve the history dependence of the continuous operator. Grünwald-Letnikov approximations provide direct difference representations, while L1-type schemes are widely used for Caputo derivatives because of their simple weighting structure and compatibility with conventional time-stepping methods.

On a uniform temporal grid $t_n = n\Delta t$, let $c^n = c(x, t_n)$, with the spatial dependence omitted from the discrete temporal formula. For $0 < \alpha < 1$, the L1 approximation is:

$$
\begin{gathered}
{}^{C}D_t^{\alpha} c^n \approx \frac{1}{\Gamma(2-\alpha)(\Delta t)^{\alpha}} \sum_{k=0}^{n-1} b_k \left(c^{n-k} - c^{n-k-1}\right), \\
b_k = (k+1)^{1-\alpha} - k^{1-\alpha}, \;\; 0 < \alpha < 1
\end{gathered}
\tag{19}
$$

The discrete convolution weights account for the contribution of all previous increments. For sufficiently smooth solutions, the L1 formula has a nominal temporal accuracy of order $2 - \alpha$ [143]. Fractional evolution problems, however, often have reduced regularity near the initial time, even when the prescribed data are smooth, and the observed convergence order can therefore be considerably lower. Graded meshes, starting corrections, singularity subtraction, and nonuniform quadrature can improve accuracy by resolving or compensating for the initial layer [144, 145]. Higher-order alternatives include $L2$-type and $L2$-1_{σ} formulas, as well as convolution-quadrature methods based on backward differentiation or Runge-Kutta schemes [146–148]. Their relative performance depends on solution regularity, stability requirements, and compatibility with variable time steps.

For a direct history sum, the computational cost over N_t time steps grows quadratically with N_t, and the state history must be stored for every spatial unknown. Fast convolution, block-FFT methods, sum-of-exponentials approximations, recursive kernel compression, and adaptive history representations can substantially reduce these costs [149–151]. Their accuracy, however, must be assessed against the original kernel. History truncation introduces an additional source of approximation error [152], and an overly short memory window can distort the long-time power-law response. Fast algorithms developed for stationary convolution kernels may also need substantial modification when applied to variable-order formulations [153].

Time-discretization methods should therefore be evaluated in terms of kernel consistency, stability, convergence for solutions with limited regularity, preservation of positivity or maximum principles where relevant, and error over the full simulation interval. Parameter estimation introduces an additional requirement because poor resolution of the initial transient or long-time tail can bias the inferred fractional order and generalized transport coefficient. Numerical discretization error should therefore be controlled as part of the inverse problem rather than treated separately from parameter recovery [154]. These considerations define the temporal part of the numerical problem; the discretization of spatially nonlocal operators is considered next.

4.4. Numerical treatment of space-fractional operators

The numerical treatment of spatial fractional operators depends strongly on how the operator is defined and on the domain over which it acts. Directional Riemann-Liouville or Riesz derivatives on regular grids are often approximated using shifted Grünwald formulas, finite differences, or finite-volume schemes. Integral fractional Laplacians require quadrature over extended spatial interactions, while spectral fractional Laplacians are commonly evaluated using eigenfunction expansions, matrix functions, or extension formulations. A numerical method developed for one operator definition does not generally approximate another, even when both use the same fractional order [155, 156].

For the integral fractional Laplacian with zero exterior data, a representative weak formulation is written in terms of the bilinear form:

$$a_\beta(u, v) = \frac{C_{d,\beta}}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{[u(x) - u(y)]\,[v(x) - v(y)]}{|x - y|^{d+\beta}} dy\, dx, \quad 0 < \beta < 2 \tag{20}$$

where u and v vanish in $\mathbb{R}^d \setminus \Omega$. Finite-element discretization of this weak form can accommodate irregular geometries, but the nonlocal interaction between basis functions generally leads to dense stiffness matrices. Accurate quadrature must also resolve both the kernel singularity and contributions from the exterior domain. Because the solution may have limited regularity near the boundary, mesh grading or adaptive refinement can be important for recovering the expected convergence behavior [157, 158].

Finite-difference methods are efficient on structured grids and can produce Toeplitz or related matrix structures that support fast solution algorithms [159]. Spectral methods can achieve high accuracy for sufficiently smooth solutions and simple geometries, while matrix-transfer and rational-approximation techniques evaluate fractional powers of discrete local operators without explicitly forming the full fractional matrix [160]. Extension methods reformulate selected fractional Laplacians as local problems in a higher-dimensional domain, replacing spatial nonlocality with an additional coordinate and a degenerate weight. Finite-volume formulations are useful when discrete conservation is a priority, although defining a physically meaningful nonlocal flux still requires careful treatment [161].

Computational acceleration can be achieved using fast Fourier techniques, hierarchical and low-rank matrix approximations, preconditioning, and multigrid methods [162–164]. However, efficiency alone is not enough. Any compression or truncation strategy must preserve the kernel, exterior interactions, symmetry or directional bias, and the conservation properties of the chosen operator. Verification should therefore include convergence in a norm appropriate to the operator, together with checks on mass balance, positivity, boundary behavior, and asymptotic spreading.

4.5. Numerical methods for coupled and nonlinear fractional models

Coupled fractional models combine memory or spatial nonlocality with reaction, thermal, electrical, mechanical, or fluid transport processes. Their numerical complexity comes not only from the cost of evaluating fractional operators, but also from interactions among fields with different characteristic scales, nonlinear constitutive relations, and interface conditions [165, 166]. As discussed in Section 3.6, applying fractional operators to the accumulation term, flux law, or kinetic relation represents different constitutive assumptions. The numerical formulation must preserve these distinctions rather than shift memory effects between equations simply for computational convenience.

Monolithic methods solve all coupled fields within a single algebraic system and can maintain strong consistency between the coupled components, but they often lead to large, dense, and poorly conditioned systems. Partitioned or staggered methods solve the individual fields sequentially, which reduces implementation complexity and allows existing solvers to be reused. Their accuracy depends on the strength of the coupling, the iteration tolerance, and any temporal lag introduced between subsystems [167]. Operator-splitting methods provide a related form of decomposition, although splitting errors can become significant when the separated operators do not commute [168, 169]. Conservation across interfaces and the consistent transfer of history-dependent variables must therefore be checked explicitly.

Implicit-explicit schemes typically treat stiff transport or reaction terms implicitly while evaluating less restrictive terms explicitly. Their efficiency depends on whether the chosen partition maintains stability and positivity [170]. Nonlinear systems can be solved using Picard iteration, Newton methods, Jacobian-free Newton-Krylov algorithms, or nonlinear multigrid. For example, Newton-based finite-element schemes have been applied to time-fractional nonlinear diffusion equations [171]. Additional difficulties arise when diffusivities, fractional orders, or memory kernels depend on the state because the operator then changes as the solution evolves. In nonlinear variable-order formulations, the fractional order may itself depend on the evolving solution [172]. In such cases, previously computed history weights or matrix factorizations may no longer be reusable, and the linearization must account for the dependence of the nonlocal operator on the current state.

Robust algorithms should be assessed using more than residual reduction alone. Relevant tests include convergence of the coupling iterations, sensitivity to operator splitting and time-step size, preservation of mass and energy balances, positivity of transported quantities, and recovery of the appropriate classical limits. Manufactured solutions and simplified one-way-coupled cases can help isolate implementation errors before the full multiphysics system is considered. Because repeated solution of these models can remain too expensive for inverse analysis or real-time prediction, the next subsection considers data-driven surrogates and hybrid computational approaches.

4.6. Data-driven and hybrid computational approaches

Data-driven methods can contribute to fractional transport modeling in four main ways: accelerating repeated forward simulations, solving inverse problems, learning unresolved constitutive components, and building reduced-order representations. Surrogate regression, reduced-basis models, Gaussian-process emulators, and neural operators approximate the relationship between model inputs, such as parameters, initial or boundary data, and material descriptors, and the resulting transport fields or observables. Their main advantage appears in many-query applications, including optimization, uncertainty propagation, and parameter estimation, where the cost of generating training data can be offset by much faster subsequent evaluations [173–175].

Physics-informed neural networks combine the governing equation, initial and boundary conditions, and observational data within a single training objective. For fractional equations, however, automatic differentiation does not eliminate the computational cost associated with nonlocal operators. Evaluating fractional residuals still generally requires quadrature, discrete convolution, spectral approximation, or stochastic treatment of the underlying operator. Fractional physics-informed neural networks are therefore better viewed as hybrid numerical-learning methods than as purely mesh-free replacements for conventional discretization [176]. Their performance also depends on the choice of collocation points and on how singular behavior is handled, particularly when temporal memory and spatial nonlocality are present together. Residual weighting and optimization dynamics can further influence the training process [177].

Neural operators and related architectures learn mappings between function spaces and can serve as surrogates across families of coefficients, source terms, geometries, or operating conditions [178]. More recent operator-learning frameworks have also been extended to families of fractional PDEs with fixed or variable fractional orders [179]. Once trained, these models can be computationally efficient, but their reliability depends strongly on the coverage and quality of the training data. Performance outside the sampled ranges of parameters, geometries, fractional orders, or forcing conditions should therefore not be assumed. More broadly, studies of operator learning under conditional shift show that changes in geometry or model dynamics require explicit testing of transfer performance [180]. Comparisons with conventional solvers should also account for the offline costs of data generation and training rather than focusing only on inference speed.

Hybrid constitutive models offer a more targeted use of learning. A fractional governing equation can retain conservation and known transport structure while a data-driven component estimates a state-dependent coefficient, fractional order, memory kernel, or microstructure-to-parameter relationship [181]. The hybrid constitutive strategy may improve flexibility without abandoning physical interpretation, but it can also increase structural nonuniqueness. For example, Coelho et al. demonstrated non-uniqueness of the optimized fractional order when the order and neural-network component were learned jointly [182]. Independent constraints, regularization, uncertainty analysis, and out-of-distribution validation are therefore essential.

Data-driven methods should ultimately be judged by the same standards as conventional solvers, supplemented by tests of training stability, generalization, reproducibility, and uncertainty calibration. Agreement with training data is not equivalent to numerical convergence or physical validation. Uncertainty arising from limited data, network hyperparameters and overparameterization, optimization, sampling, and model misspecification should also be distinguished from physical parameter uncertainty [183]. The verification principles required for both conventional and learned fractional solvers are examined next.

4.7. Stability, convergence, and numerical verification

Numerical verification determines whether a computational method solves the specified fractional model correctly; it is distinct from validating that model against physical observations [184]. Consistency requires the discrete temporal or spatial operator to approach the selected continuous operator under mesh refinement. Stability requires perturbations from data, roundoff, iteration, or previous time levels to remain controlled over the simulation interval. Convergence then depends on consistency and stability, together with the regularity of the exact solution and the function space associated with the operator.

These requirements are more demanding for fractional equations than for comparable local models. Time-fractional solutions often develop weak singularities near the initial time, which can reduce the accuracy of schemes derived under smoothness assumptions [185]. Space-fractional solutions may likewise exhibit limited regularity near the boundary even when the forcing and geometry are smooth [186]. Stability and error analyses therefore rely on tools tailored to the operator, including positivity and monotonicity of convolution weights, discrete energy estimates, generating-function arguments, and comparison principles. Discrete fractional Grönwall inequalities provide an additional framework for establishing stability and convergence [187]. Any reported convergence order should therefore be accompanied by the assumed solution regularity, temporal mesh, spatial operator, and boundary or exterior conditions.

Verification should follow a clear hierarchy. Analytical and semi-analytical solutions provide the strongest benchmarks when they use the same operator and domain as the numerical model. Manufactured solutions are valuable for more complex cases [188], but the source term, history, and exterior data must be constructed consistently with the nonlocal operator. Temporal and spatial resolutions should first be refined separately before combined refinement is examined. Fast-history tolerances, kernel-compression rank, iterative-solver tolerance, nonlinear-coupling tolerance, and surrogate approximation error should also be varied independently so that the different sources of numerical error can be distinguished.

Standard norm-based errors remain useful, but they may not capture the transport features that matter most physically. Verification should also examine conservation, positivity, maximum principles where relevant, initial and boundary behavior, long-time decay, and anomalous spreading rates. For heavy-tailed spatial solutions, conventional moments may be undefined [189] or, on finite computational domains, strongly influenced by domain truncation. In such cases, quantiles, tail exponents, truncated moments, or the mass contained within prescribed regions may provide more informative diagnostics. Learned surrogates require additional testing across unseen parameters, forcing conditions, and geometries, together with checks for reproducibility across different training realizations.

A numerically verified solver is essential for reliable parameter inference because discretization or approximation errors can otherwise be absorbed into the estimated fractional order or generalized transport coefficient [190]. The following subsection, therefore, turns to parameter identification only after separating numerical error from constitutive information. **Table 1** summarizes selected computational approaches discussed in Sections 4.2–4.7, comparing their main applications, computational structure, principal limitations, and essential verification requirements. No single computational approach is best suited to every fractional transport problem. The choice of method depends on the operator definition, computational domain, solution regularity, geometry, required physical properties, and the intended use of the model.

Table 1. Comparative characteristics of selected computational approaches for fractional transport equations.

Method family	**Primary application**	**Main computational feature**	**Principal limitation**	**Essential verification**
Transform and eigenfunction methods	Linear benchmark problems	Semi-analytical reference solutions	Simple geometries and coefficients	Transform inversion and asymptotic behavior
L1 and convolution-quadrature schemes	Time-fractional evolution	Direct approximation of temporal memory	History cost and initial singularities	Temporal refinement and long-time accuracy
Fast-memory algorithms	Long-duration time-fractional simulation	Compressed or accelerated history evaluation	Additional kernel-approximation error	Comparison with the uncompressed kernel
Grünwald, finite-difference, and finite-volume methods	Directional or Riesz-type spatial models	Efficient on structured grids	Operator- and boundary-dependent consistency	Conservation, positivity, and grid refinement
Finite-element and integral methods	Irregular geometries and bounded nonlocal domains	Flexible geometry and weak formulation	Dense coupling and singular quadrature	Operator-specific norms and exterior-data treatment
Spectral and matrix-function methods	Spectral fractional operators	High efficiency for compatible geometries	Limited geometry and operator flexibility	Eigenvalue resolution and boundary consistency
Data-driven and surrogate methods	Repeated forward or inverse calculations	Low online evaluation cost after training	Training dependence and weak extrapolation guarantees	Out-of-distribution testing and comparison with verified solvers

4.8. Parameter identification and inverse problems

Fractional transport parameters are usually inferred rather than measured directly. The unknown parameter vector may contain temporal or spatial fractional orders, generalized transport coefficients, reaction parameters, source terms, initial or boundary quantities, and parameters associated with variable-order functions or memory kernels. Experimental observations may include transient fields, breakthrough curves, frequency-domain responses, images, or integrated quantities such as terminal voltage, effluent concentration, and average temperature. An observation operator is therefore needed to relate the simulated state to the quantity that can be measured experimentally [191].

A regularized deterministic inverse problem can be expressed as:

$$\widehat{\theta} = \arg\min_{\theta\in\Theta} \left[\ \|\mathcal{H}\left[c(\theta)\right] - y^{*}\|_{W}^{2} \ + \lambda\mathcal{R}(\theta)\right] \tag{21}$$

where θ denotes the parameter vector, $c(\theta)$ is the forward-model solution, $\mathcal{H}$ is the observation operator, y^{*} represents the measurements, W specifies their weighting, and $\mathcal{R}$ is a regularization term with strength λ. The admissible set Θ should restrict the parameters to physically and mathematically meaningful ranges, including dimensional consistency when generalized coefficients depend on the fractional order [192].

Identifiability should be evaluated before any physical meaning is assigned to the estimated parameters. Structural identifiability asks whether exact, continuous, noise-free observations would uniquely determine the parameters for the assumed model. Practical identifiability concerns whether the available finite and noisy measurements contain enough information to distinguish them reliably. Fractional orders and generalized transport coefficients are often strongly correlated, and further ambiguity can arise from uncertain initial conditions, boundary forcing, source terms, or instrument response. Over a limited measurement window, a fractional model may also be observationally indistinguishable from a multirate or heterogeneous classical model. A narrow confidence interval returned by an optimizer, therefore, does not, by itself, resolve structural ambiguity [193, 194].

Estimation methods include gradient-based and derivative-free optimization, adjoint and sensitivity approaches, maximum-likelihood estimation, and Bayesian inference. However, none of these methods establishes parameter identifiability on its own. Published studies illustrate the difference between parameter estimation and parameter identifiability. Aghdam et al. examined the structural identifiability of a fractional-order impedance model containing two constant-phase elements and a Warburg term using coefficient mapping, and showed that data length and sampling time influence the numerical identifiability assessment [128]. Jacob et al. applied particle Markov chain Monte Carlo inference to fractional-order battery models using both experimental and synthetic data, demonstrating the influence of record length, excitation magnitude, prior information, and measurement noise on practical parameter recovery [195]. In time-fractional heat conduction, Zhuang et al. estimated the Caputo order from experimental carbon–carbon composite data using the Levenberg–Marquardt method and supplemented the inversion with sensitivity analysis [196]. The inverse-problem examples demonstrate that an accurate calibration does not establish parameter uniqueness; structural analysis, sensitivity assessment, or uncertainty characterization is required before fitted fractional parameters are assigned constitutive meaning.

Experimental design is therefore integral to parameter identification. Measurements should span the temporal, spatial, or frequency ranges over which the fractional parameters have distinguishable effects and, where possible, should combine complementary observables or operating conditions [197]. Synthetic inverse tests should also avoid using the same discretization to generate and recover the data, since the resulting inverse crime can hide numerical and structural errors. Ultimately, the inferred parameters should be tested against observations and conditions that were not used for calibration. The next subsection considers the remaining uncertainty and whether a fractional model is preferable to competing formulations.

4.9. Uncertainty quantification and model discrimination

Uncertainty in fractional transport modeling comes from several distinct sources. Parametric uncertainty reflects incomplete knowledge of fractional orders, generalized coefficients, source terms, and other constitutive quantities. Observational uncertainty arises from measurement noise, sampling limitations, and uncertainty in the observation operator. Numerical uncertainty is introduced through discretization, iterative solution, kernel compression, and surrogate approximation. Structural uncertainty concerns the governing model itself, including the choice of fractional operator, kernel, boundary formulation, and competing non-fractional descriptions. Focusing only on parameter uncertainty while holding all other modeling choices fixed can therefore lead to unrealistically narrow predictions [198].

The constitutive criteria developed in Section 3.7 identify which candidate models are physically plausible, while model discrimination asks whether the available observations contain enough information to distinguish among them.

A Bayesian formulation can represent uncertainty both within and across candidate models:

$$p\left(\theta, M|y^*\right) \propto p\left(y^*|\theta, M\right) p\left(\theta|M\right) p(M) \tag{22}$$

where M denotes the model class, θ its parameters, y^* the observations,$p\left(y^* \mid \theta, M\right)$ the likelihood, and $p\left(\theta \mid M\right)$ and $p(M)$ the parameter and model priors. Integrating over θ gives the model evidence, which can be used to compare candidate models or construct model-averaged predictions [199,200]. However, these comparisons depend on the choice of priors, likelihood assumptions, numerical error, and model discrepancy, so Bayesian evidence should not be interpreted automatically as proof of physical validity.

Model discrimination should involve credible alternatives rather than comparing a fractional equation only with its classical limit. Depending on the application, candidate models may include heterogeneous local formulations, multirate or mobile-immobile models, distributed relaxation networks, stretched-exponential kinetics, tempered or variable-order fractional equations, and coupled time-space fractional models. Published comparisons show why this broader benchmarking is important. Brociek et al. compared classical and fractional heat-conduction models against temperature measurements in porous aluminum, while Guerra et al. found that the identified fractional order approached the integer-order limit ($\alpha = 1.0$) and that the classical ODE baseline produced lower error when frozen parameters were transferred to held-out cells [123,201]. A better calibration fit alone is not enough because a more flexible model may fit noise or compensate for incorrect boundary conditions. Information criteria, likelihood ratios where their assumptions are satisfied, Bayes factors, cross-validation, and posterior predictive checks can provide complementary statistical evidence [127,202], but none of these methods replaces mechanistic assessment.

Predictive testing should rely on data that were not used for parameter estimation and, where possible, should involve changes in geometry, boundary forcing, operating regime, specimen, or observation scale. Randomly withholding individual time points often provides only weak evidence when neighboring observations are strongly correlated, whereas withholding entire experiments or operating conditions offers a more demanding test of transferability [203]. The stability of the inferred fractional parameters across these tests is also informative. Large, unexplained parameter shifts may indicate that the model is acting as a condition-specific surrogate rather than as a transferable constitutive description.

Uncertainty should ultimately be propagated to the quantities that inform scientific or engineering decisions and reported as intervals or distributions rather than as point estimates alone. A defensible fractional model should remain predictive under new conditions, compare favorably with plausible alternatives, and retain parameter values that are consistent with independent physical evidence. Experimental and physical validation provide the final stage of model assessment.

4.10. Experimental validation and physical consistency

Experimental validation examines whether a numerically verified and calibrated model represents the physical system accurately enough for its intended purpose. Agreement with calibration data is necessary, but it is not sufficient, especially for fractional formulations whose flexible kernels and orders can reproduce a broad range of non-exponential or heavy-tailed responses. Validation should therefore consider both predictive performance and whether the selected operator is consistent with independent evidence about the underlying transport mechanism.

Within the framework adopted in this review, experimental validation is assessed through three cumulative levels of evidence: phenomenological representation, mechanistic support, and predictive transferability.

Phenomenological validation determines whether the model can reproduce measured fields or observables, including their transient, asymptotic, spatial, or frequency-dependent behavior. The assessment should consider residual structure and uncertainty-aware metrics rather than relying on a single goodness-of-fit statistic. Where possible, multiple observables should be used because an integrated response can hide compensating errors among transport coefficients, fractional orders, source terms, and boundary conditions. For example, Kang et al. evaluated a time-space fractional subdiffusion model against gas adsorption-desorption experiments on heterogeneous coal samples and compared its performance with Fickian diffusion-based models [101].

Mechanistic validation asks whether the inferred fractional behavior is supported by evidence that is independent of the calibration data. Relevant evidence may come from residence-time or displacement statistics, relaxation spectra, microstructural imaging, connectivity analysis, tracer measurements, or direct observations of trapping and release. Such information can help distinguish temporal memory from spatial nonlocality and can test whether the assumed kernel, jump process, or variable-order dependence is physically plausible. Mechanistic support does not require every microscopic process to be resolved, but the evidence should be compatible with the constitutive interpretation assigned to the fractional operator. Mashayekhi et al., for example, related fractional viscoelastic and thermal-diffusion behavior in elastomers to independently characterized fractal structure, providing evidence beyond response fitting alone [204].

Transfer validation provides the most demanding assessment. Parameters identified under one condition should, where possible, be tested without complete recalibration under changed forcing, geometry, specimen, material state, or operating regime. Published studies provide useful examples of cross-condition validation, although relatively few satisfy the requirement for transfer without complete recalibration. Wang et al. developed temperature-compensated fractional-order models for lithium-ion batteries and ultracapacitors and evaluated their responses under dynamic operating cycles at different temperatures [205]. Kang et al. tested a fractional heat-conduction model for gas adsorption in coal under three different initial-pressure conditions and found that the same fractional order, $\alpha = 0.86$, reproduced the measured heat-flux behavior across all three experiments more accurately than the Fourier-law model [206]. These results provide evidence of parameter consistency across changed operating conditions, but they do not establish universal transferability across materials, geometries, or observation scales. Transferability should therefore be judged over the range for which the model is intended, and parameter changes should be interpreted rather than absorbed automatically through refitting. Failure under changed conditions may indicate an omitted mechanism, scale dependence, structural evolution, or an operator that is valid only over the original observation window.

Physical consistency should be evaluated alongside predictive accuracy. The complete model must satisfy the relevant conservation laws, dimensional requirements, causality, admissible initial and boundary behavior, nonnegativity of physically constrained quantities, and recovery of the appropriate classical limits. Thermodynamic compatibility, including nonnegative dissipation where relevant, should be demonstrated for the coupled constitutive system rather than assumed from the fractional operator alone.

Reproducibility also depends on clearly reporting the operator definition, kernel, domain, boundary and exterior data, numerical tolerances, calibration interval, uncertainty assumptions, and parameter units, together with accessible data and code where feasible.

A fractional transport model becomes scientifically convincing only when numerical verification, identifiable calibration, uncertainty-aware model discrimination, and experimental validation provide consistent support. This integrated verification, identification, discrimination, and validation framework forms the basis for evaluating the materials and energy applications discussed in Section 5.

5. Applications in materials and energy systems

5.1. Evaluating fractional transport models in real systems

Applications provide the clearest test of whether fractional transport models offer more than mathematical flexibility. In materials and energy systems, their use is often motivated by observations of non-Fickian spreading, non-exponential relaxation, distributed impedance response, and transport coefficients that change with scale or operating state [4, 13, 207]. These observations can motivate reconsideration of local integer-order constitutive laws, but they do not uniquely establish a fractional mechanism. Comparable responses may also result from heterogeneous classical coefficients, multirate exchange, distributed kinetics, evolving boundaries, or measurement effects [4,13,14].

The applications reviewed below are assessed using the three levels of evidence established in Section 4.10: phenomenological representation, mechanistic support, and predictive transferability. Phenomenological representation concerns whether the model reproduces the observed transport behavior. Mechanistic support requires independent evidence linking the selected operator, kernel, or fractional order to plausible microstructural or stochastic processes. Predictive transferability examines whether parameters calibrated under one condition remain meaningful when the forcing, geometry, specimen, material state, or observation scale changes. The three levels are cumulative: successful representation can establish phenomenological usefulness without necessarily demonstrating the underlying mechanism or transferability.

The strength of an application is therefore judged by the transport evidence supporting fractionalization, the definition and placement of the fractional operator, parameter identifiability, comparison with plausible fractional and non-fractional alternatives, and validation beyond the calibration data [10, 13, 123, 128]. The three-level evidence framework further helps distinguish mature application areas from emerging uses where fractional formulations remain exploratory. The following subsections apply these criteria to porous and heterogeneous materials, electrochemical systems, thermal transport, subsurface energy systems, reactive processes, and engineered functional materials.

5.2. Porous and heterogeneous materials

Porous materials offer a physically plausible setting for fractional transport because trapping, dead-end pores, connectivity bottlenecks, adsorption, and exchange between mobile and weakly mobile regions can generate broad transport timescales. Continuous-time-random-walk descriptions provide one mechanistic route from unresolved heterogeneity to time- or space-fractional transport equations, although heterogeneous local and multirate models can produce similar macroscopic behavior. Laboratory studies show both the usefulness and the limits of this interpretation. Tempered fractional models, for example, have reproduced late-time bromide breakthrough in repacked sand columns, with inferred parameters changing with grain-size distribution and flow velocity. However, a unique relationship between those parameters and independently measured pore structure has not yet been established [208,209].

Cementitious materials provide a more application-specific example. Chloride penetration in reinforced concrete has been modeled using multi-term time-fractional diffusion equations with parameters estimated from measured concentration profiles. Caputo models have also been evaluated for concrete containing fly ash or slag and compared directly with classical Fickian diffusion. These studies report improved representation of time-dependent chloride penetration and demonstrate the practical use of fractional inverse modeling [210, 211]. However, they do not establish a single fractional order as an intrinsic material property because chloride binding, saturation, cracking, pore refinement, and spatial variations in diffusivity can produce similar apparent memory effects.

Experimental studies in other heterogeneous solids lead to a similar conclusion. Methanol transport through ZSM-5 zeolite pellets has been examined using classical diffusion, time-fractional diffusion, and fractional-Brownian-motion formulations. The Fickian model was inadequate for the measured transport kinetics, whereas both anomalous models reproduced the observations, allowing alternative non-Fickian mechanisms to be compared rather than assuming a single fractional description from the outset [212]. In three-dimensional woven composites exposed to hydrothermal conditions, a two-stage time-fractional model has also reproduced experimentally measured non-Fickian moisture uptake [213]. These models can provide compact macroscale descriptions of distributed pathways and relaxation times, but agreement with bulk transport measurements alone does not reveal whether the fitted fractional parameters reflect pore connectivity, interfacial resistance, local mobility, or unresolved structural heterogeneity.

Porous and heterogeneous materials represent a comparatively well-supported application class in terms of phenomenological representation. Mechanistic support is stronger when anomalous transport can be independently related to trapping, residence-time distributions, pore architecture, or heterogeneous mobility, although direct quantitative relationships between fractional parameters and measurable microstructure remain uncommon. Establishing predictive transferability across specimens, microstructures, environmental conditions, and observation scales is more challenging. Fractional formulations are therefore most persuasive when they outperform plausible multirate, network-based, or heterogeneous classical alternatives while retaining interpretable parameters under conditions not used for calibration.

5.3. Electrochemical energy storage and conversion systems

Electrochemical devices involve ionic, electronic, thermal, and interfacial transport within porous and multiphase architectures. Fractional modeling in this area generally follows two related but distinct approaches. Fractional equivalent-circuit models employ constant-phase or generalized diffusion elements to represent distributed impedance and relaxation responses, whereas fractional governing equations modify field-level transport or kinetic laws. The extensive use of fractional circuit elements in batteries, supercapacitors, and fuel cells is well documented [6, 12], but an accurate fractional impedance model does not by itself demonstrate that concentration, potential, or temperature fields obey a fractional partial differential equation. The circuit exponent should therefore be interpreted primarily as an effective dynamic parameter unless an independent connection to the underlying transport mechanism is established.

Batteries provide the strongest experimental evidence for the reduced-order use of fractional models. Wang et al. [205] constructed fractional-order models for lithium-ion batteries and ultracapacitors from electrochemical impedance spectroscopy and identified their parameters using constrained global optimization. Validation under dynamic cycles and different temperatures produced mean relative voltage errors below approximately 4% for the batteries and 3% for the ultracapacitors. De Sutter et al. [214] examined a fractional differential battery model over the lifetime and state-of-charge range of 20 Ah NMC cells, compared its parameters with impedance measurements, and reported improved simulation accuracy relative to a conventional first-order RC model. More recently, Jiang et al. [215] compared a fractional equivalent-circuit model for commercial sodium-ion batteries with conventional 1RC and 2RC models across temperature, operating conditions, and aging states, again finding improved voltage prediction. These studies demonstrate substantial phenomenological representation and useful cross-condition validation, while also showing that the fitted parameters can evolve with temperature, state of charge, and degradation.

Parameter interpretation remains a central limitation. Structural-identifiability analysis of fractional impedance models has shown that uniqueness cannot be assumed merely because an impedance spectrum is fitted accurately [128]. In proton-exchange-membrane fuel cells, Taleb et al. identified a compact fractional impedance model from experimental frequency-domain and time-domain measurements and demonstrated its use for monitoring flooding and drying behavior [216]. Such results indicate that fractional parameters can carry diagnostically useful information, but they do not uniquely separate ionic transport, charge transfer, hydration, pore-scale gas–liquid transport, and distributed reaction effects. Independent electrochemical, structural, and transport measurements are therefore required before a circuit-order parameter is assigned a specific microscopic interpretation.

Electrochemical systems exhibit strong phenomenological representation, supported by impedance, dynamic-cycle, and aging experiments, while mechanistic support remains moderate because several distributed transport and interfacial processes can generate similar nonideal responses. Predictive transferability is also moderate: validation across temperature, state of charge, aging, or dynamic loading has been demonstrated in selected studies, but fractional parameters commonly change as the electrochemical state and material architecture evolve. Fractional formulations are therefore most valuable when they provide a demonstrable accuracy or complexity advantage over equivalent-circuit, transmission-line, porous-electrode, or other physically plausible alternatives while retaining identifiable parameters and acceptable performance outside the calibration conditions.

5.4. Thermal transport and heat conduction in complex media

Fractional thermal models are used when heat-transfer responses cannot be represented adequately by Fourier conduction with local, time-independent properties. Time-fractional formulations introduce distributed thermal memory, whereas space-fractional or other nonlocal formulations represent extended spatial interactions. The placement of the fractional operator is constitutively important because fractionalizing energy accumulation, heat flux, or both corresponds to different physical assumptions. Consequently, delayed temperature response, non-exponential relaxation, or scale-dependent apparent conductivity provides evidence of non-Fourier behavior but does not by itself identify the appropriate fractional operator.

Experimental studies demonstrate the phenomenological capability of such models. Zhuang et al. formulated a Caputo time-fractional heat-conduction model for a three-layer composite medium and estimated the fractional order from carbon–carbon experimental data using an inverse method and sensitivity analysis [196]. Brociek et al. compared three fractional heat-conduction models, involving Caputo and Riemann-Liouville derivatives, with a classical model using measured temperatures in porous aluminum [201]. Kang et al. combined a time-fractional heat equation with an adsorption-induced heat source for heterogeneous coal and reported agreement with three validation experiments [206]. These studies demonstrate that fractional formulations can reproduce thermal responses in heterogeneous materials and allow effective memory parameters to be estimated through inverse analysis. Agreement with measured temperature responses alone, however, does not establish a unique microscopic mechanism.

Model discrimination is especially important in thermal transport because fractional equations compete with several established non-Fourier theories. Cattaneo-Vernotte and phase-lag models introduce characteristic relaxation or delay times, Guyer-Krumhansl-type equations describe nonlocal and hydrodynamic effects, and ballistic-diffusive or phonon Boltzmann formulations become relevant when carrier mean free paths approach the observation scale. Recent reviews of heat conduction beyond Fourier show that these models arise from different thermodynamic or kinetic assumptions, yet they can sometimes produce qualitatively similar temperature histories. Fractionalization should therefore not be chosen simply because Fourier conduction is inadequate. The fractional model should instead be compared with physically plausible alternatives that match the material, length scale, and forcing timescale [14].

Thermal applications provide strong phenomenological representation, but the evidence for a unique constitutive interpretation is more limited. Mechanistic support is moderate because heterogeneity, interfacial resistance, distributed relaxation, phase evolution, and nonlocal carrier transport can all contribute to apparent memory effects. Predictive transferability remains limited because relatively few studies test fixed fractional parameters across different specimens, geometries, boundary conditions, and observation scales. Stronger validation therefore requires spatially or temporally resolved thermal measurements, independent material characterization, identifiability analysis, comparison with Fourier and non-Fourier alternatives, and prediction under conditions not used for calibration.

5.5. Subsurface, geological, and environmental energy systems

Fractured and heterogeneous geological formations provide one of the clearest mechanistic settings for anomalous transport. Long-tailed breakthrough, early arrival, non-Gaussian plume spreading, and scale-dependent dispersion can result from fracture channeling, matrix exchange, broad velocity distributions, preferential pathways, and trapping in low-mobility regions. Continuous-time-random-walk theory offers a general stochastic framework for describing these behaviors, with fractional transport equations arising as particular limiting cases rather than being automatically equivalent to the underlying CTRW description [4, 208]. Multirate mass-transfer, mobile-immobile, dual-porosity, discrete-fracture-network, and heterogeneous advection-dispersion models therefore remain important competing representations.

Field and reservoir studies show both the usefulness of fractional formulations and the limits of their interpretation. Benson et al. developed a radial space-fractional transport model for fractured rock and applied it to tracer data from a fractured granite aquifer [89]. The model reproduced the early bromide breakthrough that was underpredicted by a classical radial Fickian formulation, providing direct evidence that nonlocal dispersion can improve field-scale representation. Chang et al. subsequently applied a time-fractional convection–diffusion model to gas transport in heterogeneous soil and oil–gas reservoir settings, where heavy late-time breakthrough tails were not adequately captured by classical transport models; sensitivity analysis also showed distinct roles for the fractional index, convection velocity, and diffusion coefficient [217].

Geothermal reservoirs provide a particularly relevant energy application because tracer transport through connected fracture networks influences reservoir characterization and reinjection design. Suzuki et al. developed a spatial fractional advection-dispersion approach for tracer analysis in fractured geothermal reservoirs and compared its predictions with three-dimensional FRACSIM simulations [218]. The fractional model reproduced strongly anomalous long-tailed tracer responses and remained reasonably consistent across different well spacings. This provides useful evidence that fractional formulations can act as reduced-order descriptions of unresolved fracture-network transport, although agreement with a detailed numerical fracture model does not establish that the fractional parameters are unique intrinsic properties of the reservoir.

The evidence is less mature when the same framework is extended from conservative tracers or single-phase gas transport to more complex subsurface energy processes. Carbon storage, underground hydrogen storage, geothermal heat extraction, and reactive contaminant migration introduce multiphase flow, dissolution, geochemical reactions, thermal coupling, and evolving pore or fracture properties. Fractional parameters inferred from conservative tracer experiments should therefore not be transferred automatically to these processes without independent validation of the relevant effective transport statistics. Across subsurface applications, phenomenological representation is strong and mechanistic support is moderate, particularly where trapping, fracture-matrix exchange, or broad residence-time distributions are independently plausible. Predictive transferability remains limited, however, because geological observations are sparse and several competing upscaled models can reproduce the same breakthrough data.

5.6. Reactive transport, catalysis, and degradation processes

Reactive systems require particular care because delayed macroscopic behavior can arise from anomalous transport, distributed reaction kinetics, incomplete mixing, structural evolution, or interactions among these processes. A fractional transport equation, therefore, cannot be converted automatically into a physically consistent reaction-transport model by simply adding the reaction term from the corresponding Fickian equation. Bolster et al. demonstrated this explicitly for mobile-immobile systems, showing that reaction alters the effective memory structure and that a naively added reaction term can lead to substantially incorrect concentration predictions [117]. Recent reviews of non-Fickian reaction-diffusion models reach the same conclusion and distinguish formulations derived from continuous-time random walks, Lévy processes, fractal environments, Cattaneo-type transport, and Feynman-Kac approaches [16]. The placement and form of the fractional operator should therefore follow the assumed microscopic transport–reaction mechanism rather than mathematical convenience.

Porous catalysts provide a representative application. Experiments on methanol transport through H-ZSM-5/Al_2O_3 catalyst pellets have shown anomalous transport that can be described using time-fractional diffusion. Zhokh and Strizhak reported fractional exponents from catalyst-pellet measurements and investigated their dependence on pore structure; notably, experiments with different pellet porosities suggested that adsorption-related delays, rather than pore geometry alone, were important in the observed anomalous behavior [219,220]. Fractional extensions of the Thiele modulus have also been derived for space-, time-, and time-space-fractional diffusion in catalyst pellets [221]. These studies provide a connection between anomalous intraparticle transport and classical reactor-engineering quantities, but most evidence remains stronger for transport within the catalyst than for uniquely identifying the coupled reaction-memory law.

Direct reactive-transport experiments provide stronger tests of this coupling. Xu et al. investigated a bimolecular reaction between $CuSO_4$ and Na_2EDTA in heterogeneous porous media under different flow rates and degrees of particle-size heterogeneity [222]. A truncated fractional-order bimolecular reaction model reproduced the observed delayed mixing, heavy-tailed breakthrough, and subdiffusive behavior, while the experiments showed systematic dependence of the response on flow and medium heterogeneity. Such results demonstrate that fractional formulations can represent coupled transport–reaction behavior under controlled conditions, although alternative descriptions of incomplete mixing and heterogeneous local transport must still be considered before assigning the fractional order a unique mechanistic interpretation.

Degradation models introduce an additional identifiability problem because transport, reaction, interphase growth, mechanical damage, and material-state evolution may operate on overlapping timescales. López-Villanueva et al., for example, used a variable-order fractional formulation to model calendar aging of lithium-ion batteries under changing temperature and state of charge and reported improved predictive accuracy relative to its constant-order counterpart [223]. The additional flexibility, however, requires several fitted parameters and does not by itself establish the physical origin of the variable order. A particularly informative counterexample was reported by Guerra et al., who calibrated a Caputo fractional battery-aging model on two cells and tested it on two held-out cells without refitting [123].

Under this strict cross-cell protocol, the estimated fractional order approached the integer-order limit, indicating limited evidence for additional long-memory behavior in the state-of-health-versus-cycle representation. This result illustrates an important principle: fractional complexity should not be retained when identification and transfer tests indicate that a simpler model is sufficient.

The reactive, catalytic, and degrading systems show useful phenomenological representation, but their evidence base is more heterogeneous than that of porous, electrochemical, or subsurface transport. Mechanistic support remains limited because transport memory is difficult to separate from distributed kinetics, adsorption, incomplete mixing, moving interfaces, and structural evolution. Predictive transferability is also limited across the broader application class, despite stronger transfer evidence in selected degradation studies. Fractional formulations are most persuasive when the transport-reaction coupling is derived or justified from the underlying mechanism, their parameters are identifiable, and their predictions are tested against distributed-kinetic, moving-boundary, heterogeneous classical, or other physically plausible alternatives under conditions not used for calibration.

5.7. Emerging applications in smart, functional, and multiscale engineered materials

Smart and functional materials differ from the approximately fixed heterogeneous systems considered in Section 5.2 because their transport properties may change deliberately with temperature, deformation, electric field, chemical environment, or phase state. Fractional and variable-order formulations offer compact ways to represent distributed memory or transitions between transport regimes, but state dependence alone does not demonstrate fractional dynamics. In particular, allowing the order itself to vary introduces additional constitutive freedom that must be justified independently and assessed for identifiability and parsimony.

Organic semiconductor devices provide a direct transport example. Yang et al. developed a fractional drift-diffusion model in which fractional carrier-continuity equations were coupled with Poisson's equation and validated the resulting model against experimental current–voltage characteristics of an organic field-effect transistor [224]. A related study incorporated bending deformation into the fractional drift-diffusion description of a flexible organic transistor and reported improved transconductance prediction relative to a conventional drift-diffusion model, particularly in low-voltage operating regimes. These results show that fractional transport models can provide useful reduced descriptions of charge migration in mechanically responsive electronic materials. The fitted order, however, may depend on material type, boundary conditions, deformation, and device operating state, so improved electrical prediction does not by itself establish a unique microscopic transport mechanism.

Responsive polymers illustrate both the promise and the identifiability problem of state-dependent fractional formulations. Li et al. proposed a variable-order fractional model for shape-memory polymers and developed a numerical procedure for identifying the evolving order, showing that variable order can reproduce changes in memory behavior more flexibly than a constant-order model [59]. The study was primarily numerical, however, and therefore provides limited independent mechanistic validation. Stronger evidence was reported by Mashayekhi et al., who related fractional viscoelastic and thermal-diffusion behavior in two dielectric elastomers to independently characterized fractal and spectral dimensions and used Bayesian uncertainty quantification to connect the inferred fractional order with measured material structure [204]. The independent correspondence between fractional parameters and measured material structure provides an unusually direct example of mechanistic support because the fractional parameter was tested against structural information rather than being inferred solely from macroscopic response fitting.

Even with independent structural support, competing reduced descriptions remain possible. Pahari et al. subsequently showed that local fractal time derivatives and nonlocal fractional derivatives could predict the viscoelastic behavior of the same dielectric elastomers with comparable effectiveness over constant stretch-rate experiments. The comparison between local fractal and nonlocal fractional representations demonstrates that successful fractional fitting does not necessarily identify a unique constitutive representation, even when structural motivation exists.

At present, responsive and engineered materials remain an emerging application class. Phenomenological representation is moderate, with experimentally supported examples in organic electronics and multifunctional polymers. Mechanistic support is also moderate, with some studies relating fractional parameters to independently measured fractal structure, although this evidence remains limited to a small number of material systems. Predictive transferability is less established, particularly across geometries, deformation histories, stimulus levels, fabrication routes, and material families. Further studies should therefore examine deliberately varied material architectures and operating states to determine whether fractional parameters exhibit reproducible relationships with structure and transport or instead compensate for unresolved state dependence in conventional constitutive models.

5.8. Scientific contributions and current limitations of fractional transport models

The applications reviewed in Sections 5.2–5.7 show that fractional transport models have contributed across disciplines by providing a common constitutive language for memory, nonlocality, distributed relaxation, and anomalous spreading. Similar transport signatures can therefore be examined on a consistent basis across porous materials, electrochemical devices, thermal systems, geological formations, reactive media, and engineered materials. This common language has also helped connect fields that otherwise rely on different terminology and modeling traditions.

A second contribution is the ability to represent multiscale complexity in reduced form. Fractional formulations can capture broad residence-time distributions, relaxation spectra, or unresolved spatial connectivity using a relatively small number of constitutive parameters. This compact representation can lessen the need for large empirical networks, multiple exchange coefficients, or fully resolved simulations, while still supporting system-level simulation, inverse analysis, and diagnostics. Its scientific value, however, depends on whether the parameters are identifiable and whether the model preserves the conservation laws, boundary conditions, and coupling structure of the underlying transport problem.

Fractional modeling has also influenced how anomalous transport is interpreted. Departures from Fickian diffusion, Fourier conduction, or ideal electrochemical response can be viewed as possible macroscopic signatures of unresolved temporal or spatial organization rather than simply as experimental irregularities. This perspective has drawn greater attention to trapping, distributed relaxation, preferential pathways, interfacial heterogeneity, and coarse-grained microstructural effects. It does not, however, identify a unique fractional mechanism, because heterogeneous local models, multirate formulations, distributed kinetics, network models, and other generalized descriptions can reproduce similar observations.

The maturity of fractional transport modeling varies considerably across the three evidence levels used in the present review (**Figure 1**). Phenomenological representation is the most established, particularly in porous and heterogeneous materials, electrochemical systems, thermal transport, and subsurface applications, where fractional formulations have repeatedly reproduced anomalous transient, spatial, or frequency-domain responses. Mechanistic support is less mature because similar macroscopic behavior may arise from different microscopic processes or competing constitutive descriptions. Predictive transferability remains the most demanding criterion, since fitted orders and generalized coefficients can depend on specimen, geometry, operating condition, observation scale, boundary treatment, or evolving material state. The ratings in **Figure 1** represent a qualitative synthesis of the literature reviewed here rather than a statistical score. Strong denotes substantial published evidence across multiple studies or experimental conditions; Moderate denotes meaningful but incomplete or application-specific evidence; and Limited denotes sparse evidence, weak independent mechanistic confirmation, or insufficient testing beyond calibration conditions.

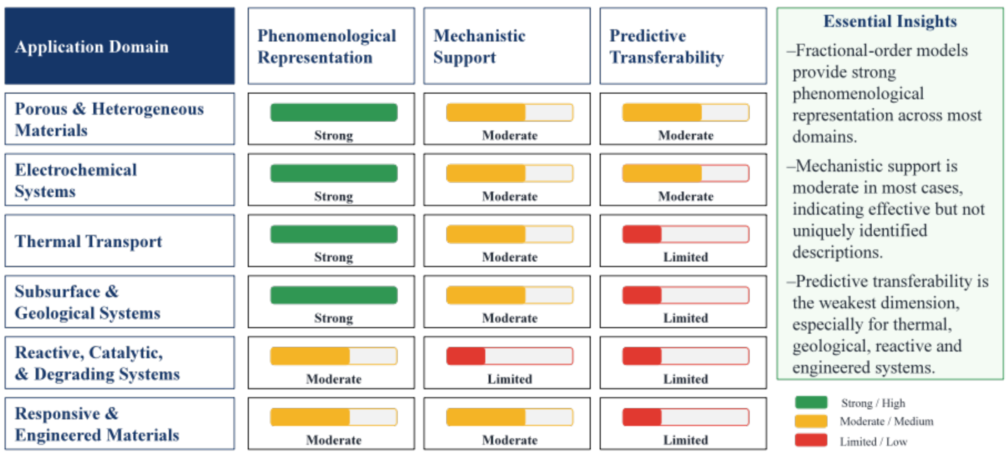

Figure 1. Cross-domain evidence assessment for fractional transport modeling in materials and energy systems. The matrix summarizes the maturity of phenomenological representation, mechanistic support, and predictive transferability across the six application domains reviewed in Sections 5.2–5.7.

The scientific interpretation of a fractional model should therefore remain proportional to the evidence supporting it. A phenomenological surrogate may be useful within a defined calibration domain without requiring a unique microscopic interpretation. A constitutive model requires, in addition, physical consistency, identifiable parameters, comparison with plausible fractional and nonfractional alternatives, and prediction beyond the calibration conditions. Strong mechanistic claims require independent evidence connecting the selected operator and its parameters to the proposed transport process. **Figure 1** summarizes the present cross-domain evidence assessment, while Section 5.9 examines the remaining requirements for advancing from successful representation toward physically grounded and transferable prediction.

5.9. Comparative perspective, unresolved challenges, and future research opportunities

The cross-domain evidence summarized in **Figure 1** shows that the maturity of fractional transport modeling remains uneven. Porous and subsurface systems have comparatively strong physical motivation because trapping, mobile-immobile exchange, preferential pathways, and broad residence-time distributions are independently plausible. Electrochemical applications offer substantial reduced-order and diagnostic value, although transport, interfacial, and kinetic contributions can be difficult to separate. Thermal models must be evaluated against established non-Fourier theories, while reactive, degrading, and responsive materials introduce further ambiguity through evolving kinetics and structure. Success in one domain, therefore, does not justify applying the same operator, parameter interpretation, or level of evidential confidence in another [4, 13, 14].

A central research priority is to determine when fractionalization is constitutively warranted rather than simply mathematically convenient. The operator definition, kernel structure, placement within the governing balance, spatial domain, and initial and boundary conditions should be consistent with the stated stochastic, microscopic, or continuum assumptions. They must also satisfy the relevant requirements for well-posedness, conservation, dimensional consistency, causality, positivity, and thermodynamic admissibility [10, 13]. This requirement becomes even more important for variable-order, distributed-order, and state-dependent models. Their additional flexibility is justified only when independent evidence supports evolving regimes or overlapping transport populations and when simpler constant-order or classical alternatives prove inadequate [9, 59].

A second priority is to connect fractional parameters quantitatively with measurable material structure. Most orders and generalized coefficients are still inferred from macroscopic responses rather than predicted from pore connectivity, tortuosity, interface density, particle-size distributions, fracture statistics, relaxation spectra, or evolving morphology. Coordinated experiments combining transport measurements with imaging, spectroscopy, tracer analysis, or microstructure-resolved simulation could determine whether fractional parameters follow reproducible structure-transport relationships [204, 225]. Such experiments should also be designed for identifiability, using complementary temporal, spatial, or frequency-domain observations and multiple forcing conditions rather than relying on a single response curve [128, 195].

Model selection must increasingly emphasize falsification and transfer rather than calibration accuracy. Fractional models should be compared with credible alternatives—including heterogeneous local, multirate, distributed-kinetic, nonlocal integral, network-based, and application-specific generalized models—under comparable data and uncertainty assumptions [4, 14]. The predictive advantage of fractional models should then be tested under changed geometry, forcing, temperature, concentration, specimen, material state, or observation scale. Public benchmark problems, experimental datasets, and reproducible computational implementations would make these comparisons far more informative. An estimated fractional order that approaches its classical limit should also be treated as a meaningful scientific result rather than as evidence of model failure. It indicates that the additional constitutive complexity is not supported under the conditions examined [123].

Multiscale simulation and data-driven methods provide a complementary path toward stronger physical grounding. Molecular, pore-network, particle-scale, and microstructure-resolved simulations can generate waiting-time, displacement, connectivity, and relaxation statistics that may be used to derive effective kernels or operators [13]. Physics-informed learning, neural operators, surrogate models, and hybrid digital-twin approaches can accelerate computation or infer relationships between material state and fractional parameters, but they should preserve the governing conservation and boundary structure, quantify uncertainty, and demonstrate predictive performance beyond the training regime [15]. The future value of fractional transport modeling, therefore, depends less on introducing additional operator families and more on developing parsimonious, falsifiable, and transferable constitutive models in which fractional structure is retained only when it provides clear physical or predictive value.

6. Conclusion

Fractional-order differential models offer a useful continuum framework for transport processes involving memory, spatial nonlocality, distributed relaxation, or multiscale heterogeneity that are not always represented adequately by conventional local constitutive laws. Their main value is not that they universally outperform classical transport models, but that they can provide parsimonious effective descriptions of unresolved temporal and spatial organization. A fractional formulation should therefore be treated as a constitutive hypothesis whose validity depends on the chosen operator, kernel, domain, initial and boundary conditions, and the physical mechanism associated with these mathematical choices. Classical integer-order models should remain the reference whenever they provide physically consistent and transferable predictions.

The evidence reviewed across porous and heterogeneous materials, electrochemical systems, thermal transport, subsurface environments, reactive and degrading media, and responsive engineered materials shows substantial but uneven maturity. Phenomenological representation generally provides the strongest evidence, with fractional models frequently reproducing long-tailed, non-exponential, non-Gaussian, or distributed dynamic responses. Mechanistic support is less consistent because similar observations can result from heterogeneous classical transport, multirate exchange, distributed kinetics, non-Fourier constitutive laws, network effects, or evolving material structure. Predictive transferability remains the most demanding criterion because fractional orders and generalized coefficients may change with specimen, geometry, operating condition, observation scale, boundary treatment, or material state.

Fractional transport is scientifically warranted when anomalous behavior is reproducible, plausible classical and generalized alternatives have been evaluated, the selected fractional operator has a defensible physical or stochastic basis, and its parameters are sufficiently identifiable. The model should also retain a predictive advantage beyond the conditions used for calibration. Additional complexity, including variable-order, distributed-order, and state-dependent formulations, is justified only when supported by corresponding evidence. The central challenge for the field is no longer to show that fractional equations can fit anomalous transport data, but to establish when they provide the simplest physically defensible and predictively transferable description of the underlying process.

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