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A Comprehensive Review of Recent Advances in Scalar Convection-Diffusion Studies

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ABSTRACT

Scalar convection-diffusion has been drawing attention in fluid mechanics since more than half a century due to its relevance in various applications, its impact on transport properties, and its interplay with other fluid phenomena. In this review, we summarize the recent advances in scalar convection-diffusion studies documented by various researchers in efforts to identify an appropriate case study for using the model of convection-diffusion correctly. Scalar convection-diffusion studies are classified as theoretical, numerical solution, extracellular, chemical reaction, turbulence, diffusivity, and mixing perspectives since different perspectives have their own context. This paper has examined and articulated a range of viewpoints with different emphases. Encapsulating the latest advancements in the study of scalar convection-diffusion processes for future case study applications is the goal of this review.

1. Introduction

The current research trend in the study of scalar convection-diffusion in fluid mechanics includes investigating buoyancy-driven convection flows using the Grossmann-Lohse theory [1]. Numerous research efforts have also concentrated on the advancement of numerical techniques aimed at addressing convection-diffusion equations [2,3] which includes analyzing semi-implicit DG schemes for scalar nonstationary nonlinear problems [3], modeling diffusive and convective transport in brain extracellular space [4], analyzing the destabilization of density stratifications by chemical reactions [5], scalar quantities evolution by molecular diffusion and turbulent convection [6], investigating double-diffusive convection flows [7,8], testing scalar solvers for convective convection-diffusion problems [9], and defining the rate of scalar mixing in fluid flows [10]. This process is relevant in various fields, including engineering, oceanography, and geophysics.

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2. Grossmann-Lohse Theory

Buoyancy-driven scalar convection flows have been studied extensively in fluid dynamics. In the study of Rayleigh-Bénard (RB) convection, Grossmann and Lohse [11] proposed that in the experimentally accessible parameter regime, the use of Prandtl and Rayleigh numbers in the formulation of pure power laws for the Reynolds and Nusselt numbers are invalid [11,12]. The regions of Grossmann-Lohse theory are shown in FigureFig. **1**. Despite more than twenty years passing since the initial claim, it still stands as a viable and applicable concept within the realm of buoyancy-driven convection flows, such as double-diffusive turbulence [7], vertical natural convection [13], axially homogeneous RB convection [14], and two-scalar turbulent RB convection [1]. A more recent extension of the Grossmann-Lohse (GL) model was made in 2021 [15] which covers tilting RB convection, horizontal convection, and magneto-convection.

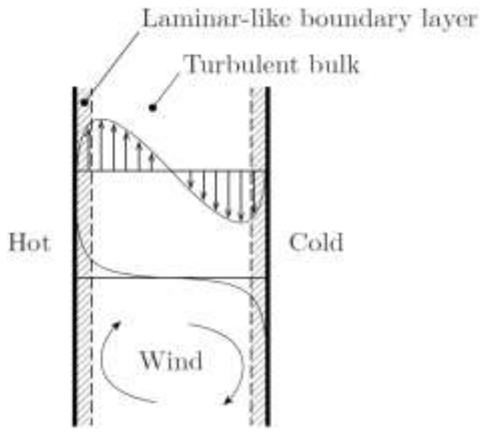


Fig. 1. Depiction of the laminar-like (boundary-layer) and turbulent (bulk) zones as described in the Grossmann-Lohse theory [13]

GL theory has been a beneficial tool for understanding buoyancy-driven scalar convection flows. Despite its applicability to a wide range of control parameters, including those relevant for ocean flows [7], the original claim does not encompass thermal convection within the high Prandtl number regime. Consequently, Wang *et al.,* [16] generalized Grossmann and Lohse's theories in offering a unifying theory for purely internally heated convection and turbulent. It is worth noting that the turbulent convective flow is frequently characterized by a significant convective structure known as a turbulent roll, commonly referred to as the wind of turbulence [17].

3. Discontinuous Galerkin Schemes

Discontinuous Galerkin (DG) methods have been demonstrated to be accurate and stable numerical approaches for approximating convection-dominated convection-diffusion problems [18]. Brdar *et al.*, [19] comprehensive study provides a detailed comparison of well-established DG methods used to solve nonlinear convection-diffusion problems. In order to model natural convection phenomena, a novel set of staggered semi-implicit DG techniques of high-order was proposed in the year 2020 [20].

The integration of DG with the widely recognized trapezoidal rule second-order backward difference formula (BDF2) [21] methods offer a powerful approach to efficiently and precisely solve partial differential equations, particularly in domains such as numerical weather prediction (NWP) and other scientific simulations. The DG-BDF2 method demonstrates adaptability, high-order accuracy, and stability, making it a valuable tool in computational science and engineering. Moreover, it serves as a benchmark for other hybridized DG methods, including those that involve hierarchical scale separation extensions [22].

To achieve the objective of addressing linear convection-diffusion-reaction problems, recent hybridized methods include advanced semi-Lagrangian DG techniques [23] of high-order, combining the accuracy and conservation properties of DG methods with the computational efficiency and robustness of semi-Lagrangian techniques. Additionally, high-order semi-implicit multistep methods have been developed for time-dependent partial differential equations, encompassing nonlinear reaction-diffusion and convection-diffusion problems [24]. These methods differ in their treatment of advection and time integration. The semi-Lagrangian DG method places emphasis on accurate and efficient advection schemes, while the semi-implicit multistep DG method prioritizes stability and robustness in temporal integration. Another variation of the semi-implicit DG method, proposed by Ioriatti *et al.,* [25], incorporates a posteriori subcell finite volume limiting technique to handle shock waves or steep gradients.

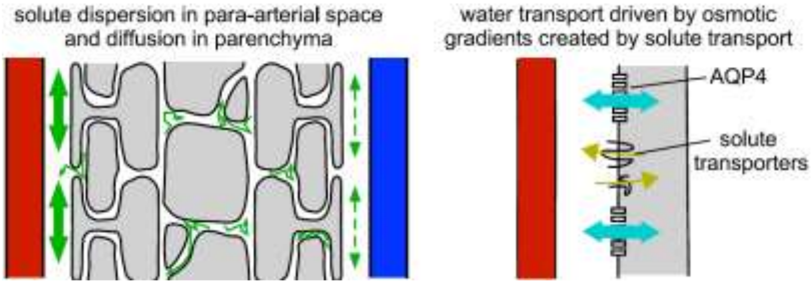
In comparison to conventional DG schemes, interior penalty DG schemes introduce penalty terms that penalize jumps in the solution and its derivative across element interfaces [26]. This penalty ensures the preservation of maximum principles at the discrete level for steady transport and convection-diffusion problems.

4. Modeling of Transport in Brain Extracellular Space

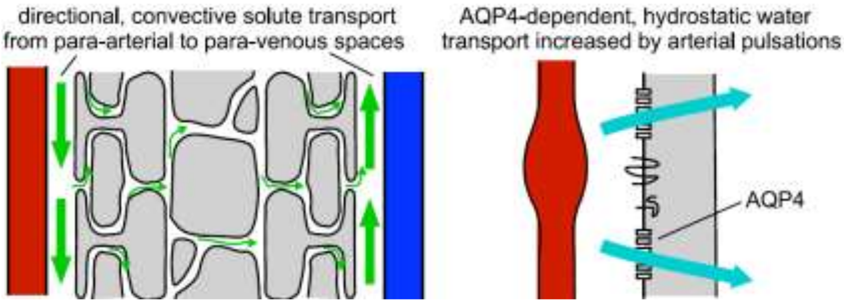
The transport of solutes in the brain particularly in its extracellular space (ECS) has been a topic interest for many years. It has been thought commonly that diffusivity and nondirectionality are the only primary characteristics of the transport of solute in brain parenchyma, particularly the narrow and tortuous extracellular space [27]. However, the transport of convection may also play a role as suggested in recent studies on the solutes transport in the brain ECS [4,27-31] as depicted in Figure Fig**. 2**.

In a study by Ray *et al.,* [28], a substantial collection of published experimental findings regarding transport mechanisms within the brain were used to verify the modeling of transport mechanisms characterized solely by diffusion, as well as the modeling of transport processes that integrate both convective and diffusive elements within the interstitial space of the brain [28]. The modellings incorporated current theories of perivascular influx and efflux as illustrated in Figure Fig**. 3** and Figure Fig**. 4**. The results of the study suggested that convective transport may play a significant role in the transport of solutes in the brain ECS. Similarly, Abbott *et al.,* [30] proposed a model that links, for clearance along peri-venous spaces, fluid delivery to venules, the aquaporin-4 (AQP4) water channel related transport of convection of solutes and fluid mediated by glia via the ECS of brain tissue, and lastly bulk of brain tissue cerebrospinal fluid (CSF) flow (i.e. that of convection) along the exterior of penetrating arteries [30]. This model suggests that convective transport may be an important mechanism for solute clearance in the brain.

However, there are also studies that suggest that diffusive transport may be the dominant mechanism for solute transport in the brain ECS [27,32-34]. For example, Smith *et al.,* [32] observed that, in a way consistent with transport of diffusion rather than that of convection, dextran size influenced dextrans fluorescent transport in brain parenchyma [32]. Similarly, Holter *et al.,* [34] found that interstitial solute transport in 3D reconstructed neuropil occurs by diffusion rather than bulk flow [34]. In conclusion, while there is evidence to suggest that convective transport may play a role in the transport of solutes in the brain ECS, there are also studies that suggest that diffusive transport may be the dominant mechanism. Further investigation into scalar convection-diffusion phenomena is imperative in order to comprehensively elucidate the intricate mechanisms behind solute transport in the brain extracellular space (ECS).



(a)



(b)

Fig. 2. Differences between conventional and contemporary perspectives (a) Conventional understanding of solute clearance [27] (b) Proposed glymphatic mechanism of solute clearance [27]

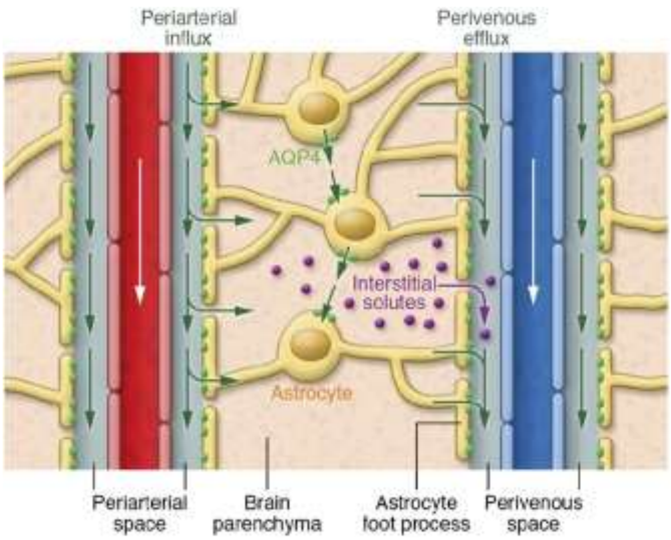


Fig. 3. The exchange occurring between the interstitial tissue (also known as parenchyma) and the perivascular space that encircles the penetrating blood vessels. Solute (represented by the purple arrow) and fluid (indicated by the green arrow) movement within brain tissue is depicted [28]

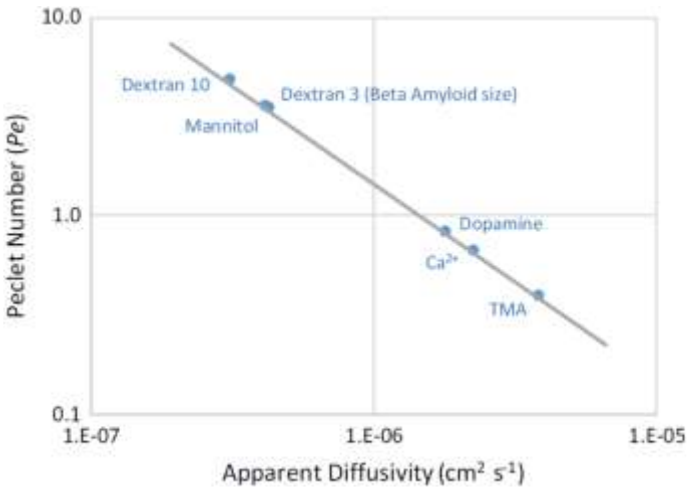


Fig. 4. The relationship between the Péclet number and the apparent diffusivity of various molecules relevant to transport within the brain [28]

5. Destabilization of Density Stratifications by Chemical Reactions

Density stratifications in scalar convection-diffusion flow can be destabilized by chemical reactions, leading to hydrodynamic instabilities. Several studies have explored this phenomenon using reaction-diffusion-convection models [5,35-38]. In addition, the phenomenon of chemical destabilization against buoyantly stable density stratifications has been the subject of numerical studies that aim to provide specific insights [39,40].

Almarcha *et al.,* [5] demonstrated in their study that density changes resulting from a simple kinetic scheme, such as $A + B \rightarrow C$, can have a significant impact on buoyancy-driven instabilities at a horizontal interface between two solutions initially containing the scalars A and B. The authors presented their findings in Figure Fig**. 5**, which clearly illustrates the effects of gravity on the system. In this particular scenario, the product C diffuses at a rate comparable to that of reactants A and B; however, it possesses a greater mass. Consequently, this leads to the emergence of a localized Rayleigh-Taylor instability, wherein the denser layer of C settles above the lighter layer of B beneath the contact line. This instability triggers convection currents, resulting in a distortion of the initially uniform reaction front. The investigation further demonstrated the development of elongated, slender fingers that extend downward from the reaction zone, while convection simultaneously elevates the reaction front. This asymmetrical behavior within the system is attributed to the stable upper stratification, where the lighter reactant A is positioned above the denser layer of C.

The stabilizing or destabilizing influence of reactions on buoyancy-driven convection has been classified in a parameter space [41], and extensively reviewed by Balakotaiah *et al.,* [42]. It is a consensus that chemical reactions might trigger convection even in cases where concentration and heat both contribute to a stable density stratification [36,37,43]. Moreover, Loodts *et al.,* [38] showed that the onset time of convection can be either enhanced or decreased by a chemical reaction, depending on the type of density profile building up in the reactive solution.

6. Scalar Quantities Evolution by Molecular Diffusion and Turbulent Convection

The study of scalar quantities evolution by molecular diffusion and turbulent convection involves the use of various mathematical models and numerical methods. Some studies focus on the analysis of convective flux density and turbulent chemical diffusivity produced by convection as a function of height [44,45]. Other studies investigate the behavior of scalar quantities in turbulent thermal convection and the intermittency of active scalar [46]. Additionally, there are studies that analyze the mixing efficiency and turbulent dissipation rate in turbulent flows [47].

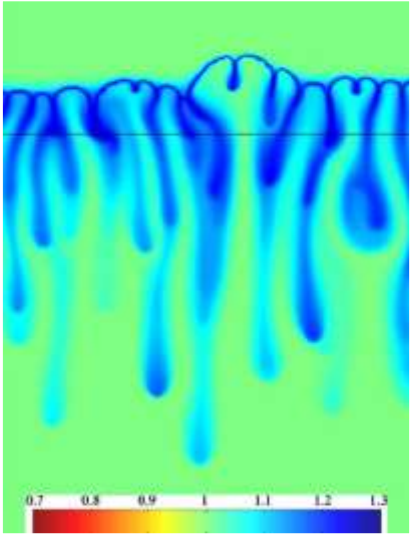


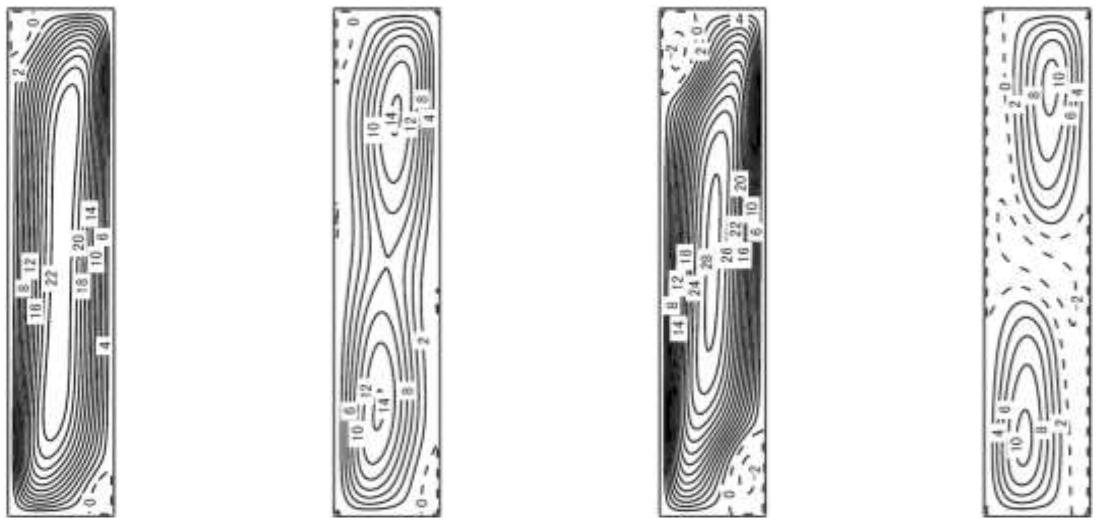
Fig. 5. 2D density fields obtained numerically, where the black line corresponds to the initial contact line [5]

7. Double-Diffusive Convection Flows

Double-diffusive convection is a hot topic since half a century [48] in research as a phenomenon that occurs when two fluids with different densities diffuse into each other, leading to buoyancy forces that drive fluid motion. The development of this field has resulted from a collaborative engagement among theorists, geophysicists, marine oceanographers, and engineers [49]. Venables *et al.,* [50] examine the potential for double-diffusive convection occurring in a scenario where cold, fresh water is situated above warmer, saline water beneath an Antarctic ice shelf. While numerous access points have been created in ice shelves to facilitate the placement of instruments for extended monitoring, this study marks the inaugural observation of the impacts of diffusive convection. Notably, a distinct thermohaline staircase is evident in both the temperature and salinity profiles.

Double-diffusive convection driven by both thermal and compositional buoyancy in a rotating spherical shell was investigated by Silva *et al.,* [51]. In a double-diffusive setup, they numerically investigated the linear onset of instability of convection. This is important in order to understand how the thermo-compositional convection dynamics is determined by the compositional and thermal molecular diffusivities differences. Another numerical analysis of double-diffusive convection was carried out by Masuda *et al.,* [52] where opposing heat and mass fluxes on the vertical solid surfaces cause the phenomena in a permeable surface. Figure **Error! Reference source not found.** reveals that the main flow is driven thermally. The upper and a lower zone of convection cell may also present due to the pattern of flow. This justifies small values of Nu since, in this case, the convection strength is weak; the concentration gradients also lead to the convection, and there is a periodically change in the pattern of convection and the velocity value. On the other hand, Nu becomes large if the flow is thermally-driven and there is only one convection cell [52].

The scope and development of the diffusive regime associated with double-diffusive convection in oceanic environments has been studied [53]. In particular, it was found that by utilizing a multifrequency acoustic backscattering technique, thin acoustic layers identified in proximity to the western Antarctic Peninsula have been found to align with scattering phenomena observed at diffusive-convection interfaces in controlled laboratory settings.



t_1 t_2 t_3 t_4

Fig. 6. Contour lines of stream functions at four different times t for Rayleigh-Darcy number $R = 100$, Lewis number $Le = 20$, buoyancy ratio $N = 0.55$, and the aspect ratio $A = 5$ [52]

More current studies include an investigation by Zaussinger and Kupka [54] of a disparity in mean molecular weight between the upper and lower layers which serves to mitigate the instability of double-diffusive convection where thermal stratification is prone to to thermal convection.

It is known that local thermal non-equilibrium regulates double-diffusive Rayleigh-Bénard convection within a dual-layered configuration. Venkatraman and Vanishree [55] examined the influence of magnetic fields on the initiation of this convection, while Manjunatha *et al.,* [56] studied Darcy-Benard double-diffusive Marangoni convection in a composite layer system with a constant heat source along with non-uniform temperature gradients.

8. Scalar Solvers

In their research, Wu and Xu introduced simplex-averaged finite element techniques specifically designed for addressing convection-diffusion challenges within the $H(\mathrm{grad})$, $H(\mathrm{curl})$, and $H(\mathrm{div})$ function spaces [57]. Their study provided compelling numerical examples that illustrated the reliability and efficiency of these methods in tackling a wide range of convection-diffusion issues. Another finite element method for convection-diffusion equations is the well-known algebraic flux correction (AFC) finite element schemes [58]. While simplex-averaged finite element methods [57] emphasize techniques like edge-averaging and exponential averaging, AFC finite element schemes [58] focus on satisfying maximum principles and entropy stability conditions.

Chertock *et al.,* [59] and Ullmann *et al.,* [60] promote the idea of breaking down the original problem into more manageable subproblems or transformed systems, which can be solved using established numerical algorithms. This decomposition or transformation approach allows for efficient computation and improved convergence behavior in solving convection-diffusion equations. Chertock *et al.,* [59] extended the fast-explicit operator splitting method for solving deterministic convection-diffusion equations to the problems with random velocity fields and singular source terms. In the solution of log-transformed random diffusion equations, Ullmann *et al.,* [60] introduced effective iterative algorithms for the stochastic Galerkin discretization. In both diffusion and convection-diffusion contexts, they conducted a comparative analysis of the performance of these iterative solvers using a model problem.

Angermann [61] made significant advancements in the field by utilizing fitted discretizations for convection-diffusion equations with scalar diffusion coefficients and extending the approach to those with anisotropic diffusion coefficients. Similarly, Patel and Dhodiya [62] extended the application of the differential transform method for reaction-diffusion to convection-diffusion problems, addressing the limitations of existing methods in the literature. These contributions have expanded the understanding and capabilities in solving convection-diffusion equations with various diffusion coefficients.

Three-dimensional convection-diffusion equations can be solved by applying the upwind Crank-Nicolson difference schemes combined with alternating bar parallelization [63] as a new solver. Such parallel unconditionally stable solver was incorporated in a Navier-Stokes solver for three-dimensional channel flow at moderately large Reynolds number [64]. In a noteworthy development, Kubrak *et al.,* [65] addressed the challenges associated with incompressible flow by integrating the discretization of the scalar convection-diffusion equation with a fourth-order Navier-Stokes solver.

9. Rate of Scalar Mixing in Fluid Flows

Scalar mixing [66] is a significant issue in convection-diffusion, with applications in environmental and industrial flows. The rate of scalar mixing in fluid flows has been extensively studied in recent years. The concept of scalar mixing is best defined in terms of the flux of the scalar across isoscalar surfaces as illustrated in Figure Fig**. 7** [10].

A remarkable philosophical viewpoint on passive scalar mixing in a diffusive fluid flow at finite Péclet number was presented by Heffernan and Caulfield [67]. Their work emphasized the fundamental nature of mixing in various environmental and industrial flows. They also proposed a robust and efficient method for identifying optimal mixing perturbations using proxy multiscale measures. Passive scalar mixing was also studied by Alqahtani *et al.,* [68], focusing on extreme events and instantons in Lagrangian turbulence models.

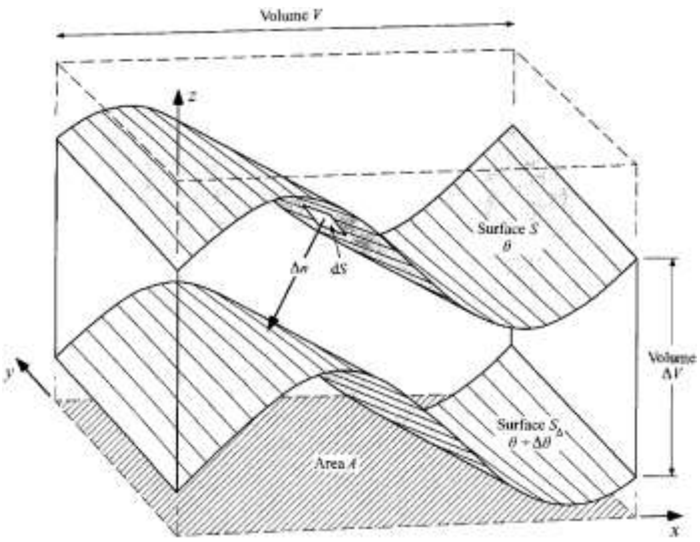


Fig. 7. Let θ and $\theta + \Delta_\theta$ are the scalar values defining the surfaces S and S_Δ, respectively, the fluid volume between such surfaces is represented by ΔV. Take a cross-section with area A in volume V, two isoscalar surfaces are possible as in this schematic [10]

The parameters that affect the rate of scalar mixing depend on the type of flow. Sreenivasan [69], for instance, discussed how a turbulently mixed state depends on the flow Reynolds number and the Schmidt number of the scalar, whereas Karasso and Mungal [70,71] investigated scalar mixing and reaction in liquid shear layers to find that the rate of scalar mixing is directly proportional to the entrainment rate and not to any hydrodynamic measures. Another example is the study three-scalar mixing in a turbulent coaxial jet by Cai *et al.,* [72] where the flow better approximates the mixing process in a non-premixed turbulent reactive flow.

Excellent examples on the validation of scalar mixing models are the work of Fox [73] and Kops and Mortensen [74], involving the use of DNS data sets. Fox proposed an efficient numerical implementation of velocity-conditioned scalar mixing for full probability density function (PDF) simulations, while Kops and Mortensen [74] provided brilliant, high-resolution description of the scalar mixing layer. Table 1 shows some scalar convection-diffusion studies.

Table 1
Scalar convection-diffusion studies

Perspective	Author
Grossmann-Lohse Theory	[1,7,11-17]
Discontinuous Galerkin Schemes	[18-26]
Modeling of Transport in Brain Extracellular Space	[4,27-34]
Destabilization of Density Stratifications by Chemical Reactions	[5,35-43]
Scalar Quantities Evolution by Molecular Diffusion and Turbulent Convection	[44-47]
Double-Diffusive Convection Flows	[48-56]
Scalar Solvers	[57-65]
Rate of Scalar Mixing in Fluid Flows	[10,52,66-74]

10. Conclusions

This paper reviewed the study of scalar convection-diffusion in fluid mechanics encompassing a wide range of research areas, including the investigation of buoyancy-driven convection flows using the Grossmann-Lohse theory, the development of numerical methods for solving convection-diffusion equations, modeling diffusive and convective transport in brain extracellular space, analyzing the destabilization of density stratifications by chemical reactions, and defining the rate of scalar mixing in fluid flows:

i) The Grossmann-Lohse theory has been instrumental in understanding buoyancy-driven scalar convection flows, with recent extensions covering various convection scenarios.
ii) Discontinuous Galerkin (DG) methods have been shown to be accurate and stable numerical approaches for approximating convection-dominated convection-diffusion problems, offering adaptability, high-order accuracy, and stability.
iii) The transport of solutes in the brain extracellular space has been a topic of interest, with evidence suggesting that both convective and diffusive transport mechanisms may play a role.
iv) Chemical reactions have been shown to destabilize density stratifications in scalar convection-diffusion flow, triggering hydrodynamic instabilities.
v) Studies have also focused on scalar quantities evolution by molecular diffusion and turbulent convection, double-diffusive convection flows, scalar solvers for convective convection-diffusion problems, and parameters affecting the rate of scalar mixing depending on the type of flow.

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