SPECTRAL ANALYSIS AND COMPUTATION OF EFFECTIVE DIFFUSIVITIES FOR TIME-DEPENDENT PERIODIC FLOWS

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Abstract. The enhancement in diffusive transport of particles or tracers by incompressible, turbulent flow fields is a challenging problem with theoretical and practical importance in many areas of science and engineering, ranging from the transport of mass, heat, and pollutants in geophysical flows to turbulent combustion and stellar convection. The long time, large scale behavior of such systems is equivalent to an enhanced diffusive process with an effective diffusivity tensor $\mathbf{D}^*$. Based on an analytic continuation method developed for random composite materials, a rigorous integral representation for $\mathbf{D}^*$ was developed for the case of a random, *time-independent* fluid velocity field, involving a spectral measure of a self-adjoint random operator acting on *vector-fields*. An alternate approach yielded an integral representation for $\mathbf{D}^*$ involving a spectral measure of a self-adjoint operator acting on *scalar-fields*, for the case of a periodic, *time-independent* fluid velocity field. Here, we adapt and extend both of these approaches to the case of a periodic, *time-dependent* fluid velocity field, with possibly chaotic dynamics, providing integral representations for $\mathbf{D}^*$ involving spectral measures of the underlying self-adjoint operators. We prove that the two approaches are equivalent and that their correspondence follows from a one-to-one isometry between the underlying Hilbert spaces. Moreover, we establish a direct correspondence between the effective parameter problem for $\mathbf{D}^*$ and that arising in the analytic continuation method for composites. We also develop novel Fourier methods that provide the mathematical foundation for rigorous computation of $\mathbf{D}^*$. Our numerical computations are in excellent agreement with known theoretical results.

Key words. advective diffusion, effective diffusivity, eddy diffusivity, spectral measure, multi-scale homogenization, turbulence, residual diffusion

AMS subject classifications. 47B15, 65C60, 35C15, 76B99 76M22 76M50 76F25 76R99

1. Introduction. The long time, large scale motion of diffusing particles or tracers being advected by an incompressible flow field is equivalent to an enhanced diffusive process [75] with an effective diffusivity tensor $\mathbf{D}^*$. Describing the associated transport properties is a challenging problem with a broad range of scientific and engineering applications, such as stellar convection [41, 66, 16, 17, 15], turbulent combustion [3, 12, 74], and solute transport in porous media [9, 10, 79, 36, 42, 45, 43]. Time-dependent flows can have fluid velocity fields with chaotic dynamics, which gives rise to turbulence that greatly enhances the mixing, dispersion, and large scale transport of diffusing scalars.

In the climate system [21, 35], turbulence plays a key role in transporting mass, heat, momentum, energy, nutrients, pollutants, and salt in geophysical flows [56]. Turbulence enhances the dispersion of atmospheric gases [23] such as ozone [38, 63, 64, 65] and pollutants [20, 8, 69], as well as atmosphere-ocean transfers of carbon dioxide and other climatically important trace gas fluxes [81, 6]. Longitudinal dispersion of passive scalars in oceanic flows can be enhanced by horizontal turbulence due to shearing of tidal currents, wind drift, or waves [80, 44, 13]. Chaotic motion of time-dependent fluid velocity fields cause instabilities in large scale ocean currents, generating geostrophic eddies [26] which dominate the kinetic energy of the ocean [27]. Geostrophic eddies [26] greatly enhance the meridional mixing of heat, carbon and other climatically important tracers, typically more than one order of magnitude greater than the mean flow of the ocean [72]. Eddies also impact heat and salt budgets through lateral fluxes and can extend the area of high biological productivity offshore by both eddy chlorophyll advection and eddy nutrient pumping [18]. In sea ice, which couples the atmosphere to the polar oceans [77], the transport of vast ice floes can also be enhanced by eddie fluxes [78]. Thermal transport through sea ice can be enhanced by a brine velocity field [47, 76], which itself depends on the brine microstructure and its connectivity [31, 32], and plays an important role in many biogeochemical processes in polar ecosystems and the climate [30].

It has been noted in various atmospheric contexts [64, 65] that eddy-induced, skew-diffusive tracer fluxes, directed normal to the tracer gradient [54], are generally equivalent to antisymmetric components in the effective diffusivity tensor $\mathbf{D}^*$, while the symmetric part of $\mathbf{D}^*$ represents irreversible diffusive effects [67, 70, 34] directed down the tracer gradient. The mixing of eddy fluxes is typically non-divergent and unable to affect the evolution of the mean flow [54], and do not alter the tracer moments [34]. In this sense, the mixing is non-dissipative, reversible, and sometimes referred to as stirring [22, 34].

Due to the computational intensity of detailed climate models [35, 77, 59], a coarse resolution is necessary in numerical simulations and *parameterization* is used to help resolve sub-grid processes, such as turbulent entrainment-mixing processes in clouds [46], atmospheric boundary layer turbulence [14], atmosphere-surface exchange over the sea [24] and sea ice [71, 1, 2], and eddies in the ocean [51, 29]. In this way, only the effective or averaged behavior of these sub-grid processes are included in the model. Here, we study the effective behavior of advection enhanced diffusion by time-dependent fluid velocity fields, with possibly chaotic dynamics, which gives rise to such a parameterization, namely, the effective diffusivity tensor $\mathbf{D}^*$ of the flow.

In recent decades, a broad range of mathematical techniques have been developed [52, 7, 11, 25, 50, 61, 62, 19, 37, 39, 48, 49] which reduce the analysis of enhanced diffusive transport by complex velocity fields with rapidly varying structures in both space and time, to solving averaged or *homogenized* equations that do not have rapidly varying data, and involve an effective parameter. Motivated by [60], it was shown [52] that the homogenized behavior of the advection-diffusion equation with a random, time-independent, incompressible, mean-zero fluid velocity field, is given by an inhomogeneous diffusion equation involving the symmetric part of an effective diffusivity tensor $\mathbf{D}^*$. Moreover, a rigorous representation of $\mathbf{D}^*$ was given in terms of an auxiliary "cell problem" involving a curl-free random field [52]. We stress that the effective diffusivity tensor $\mathbf{D}^*$ is not symmetric in general. However, only its symmetric part appears in the homogenized equation for this formulation of the effective transport properties of advection enhanced diffusion [52].

The incompressibility condition of the velocity field was used [4, 5] to transform the cell problem [52] into the quasi-static limit of Maxwell's equations [40, 33], which describe the transport properties of an electromagnetic wave in a composite medium [55]. The analytic continuation method (ACM) for representing transport in composites [33] provides Stieltjes integral representations for the bulk transport coefficients of the media, such as electrical conductivity and permittivity, magnetic permeability, and thermal conductivity [55]. This method is based on the spectral theorem [73, 68] and a resolvent formula for, say, the electric field, involving a random self-adjoint operator [33, 58] or matrix [57]. Based on [33], the cell problem was transformed into a resolvent formula involving a self-adjoint random operator, acting on the Hilbert space of curl-free *vector fields* [4, 5]. This, in turn, led to a Stieltjes integral representation for the symmetric part of the effective diffusivity tensor $\mathbf{D}^*$, involving the Péclet number of the flow and a *spectral measure* of the operator [4, 5].

The mathematical framework developed in [52] was adapted [61] to the case of a periodic, time-independent, incompressible fluid velocity field with non-zero mean. The velocity field is modeled as a superposition of a large-scale mean flow with smallscale periodically oscillating fluctuations. It was shown [61] that, depending on the strength of the fluctuations relative to the mean flow, the effective diffusivity tensor $\mathbf{D}^*$ can be constant or a function of both space and time. When $\mathbf{D}^*$ is constant, only its symmetric part appears in the homogenized equation as an enhancement in the diffusivity. However, when $\mathbf{D}^*$ is a function of space and time, its antisymmetric part also plays a key role in the homogenized equation. In particular, the symmetric part of $\mathbf{D}^*$ appears as an enhancement in the diffusivity, while both the symmetric and antisymmetric parts of $\mathbf{D}^*$ contribute to an effective drift in the homogenized equation. The effective drift due to the antisymmetric part is purely sinusoidal, thus divergence free [61]. Based on [9], the cell problem was transformed [61] into a resolvent formula involving a self-adjoint operator, acting on the Sobelov space [53, 28] of spatially periodic scalar fields, which is also a Hilbert space. This, in turn, led to a discrete Stieltjes integral representation for both the symmetric and antisymmetric parts of $\mathbf{D}^*$, involving the Péclet number of the flow and a *spectral measure* of the operator.

Here, we adapt and extend both of these approaches to the case of a periodic, *time-dependent* fluid velocity field, with possibly chaotic dynamics, providing integral representations for $\mathbf{D}^*$ involving spectral measures of the underlying self-adjoint operators. We prove that the two approaches are equivalent and that their correspondence follows from a one-to-one isometry between the underlying Hilbert spaces. Moreover, we establish a direct correspondence between the effective parameter problem for $\mathbf{D}^*$ and that arising in the analytic continuation method for composites. We also develop novel Fourier methods that provide the mathematical foundation for rigorous computation of $\mathbf{D}^*$. Our numerical computations are in excellent agreement with known theoretical results. FINISH THIS PARAGRAPH WHEN THE REST OF THE PAPER IS FINISHED.

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