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A Fundamental Solution for an Advection Diffusion Equation in a Non Uniform Three Dimensional Flow

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A Fundamental Solution for an Advection Diffusion Equation in a Non Uniform Three Dimensional Flow

Soha Al Hajj Ali

ABSTARCT

We propose in this thesis an analytical solution for the three dimensional Eulerian advection diffusion equation of a scalar tracer transported by a turbulent flow where the mean flow is assumed to be linear in space relative to the center of the patch and where the effects of the small scale eddies are resolved by introducing an effective eddy diffusivity. We show how our solution is obtained by transforming it into a system of equations for the trajectories and for the concentration in the Lagrangian frame. An apparent diffusion coefficient that combines the effects of the advection and the turbulent diffusion is inferred from the solution and some asymptotic behaviors of the diffusion are explored.

keywords: mutli-dimensional advection diffusion, turbulent flow, eddy diffusivity, apparent coefficient of diffusion

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Chapter One

Introduction

A core issue in studying ocean dynamics is to estimate the dispersion of pollutants in the ocean in order to predict their trajectories and minimize their damage on marines lives. Pollutants harm the marine ecosystem and endanger many living beings, from the smallest to the largest creature. Marine pollution can be due to chemical contamination or trash related pollution. In the latter category, plastic waste is the most common in our seas, as they hold toxic chemical agents that need hundreds of years to terminate. In particular, micro-plastics can be digested by marine species, endanger their lives, and threaten the whole food web [13] [4]. Circular currents, or eddies, are ocean structures that can transport masses of water, trap or advect for long distances water content, be it pollutants or nutrients. This has a direct impact on the biological and geo-chemical properties of water, especially in the redistribution of nutrients or the dispersion of pollutants [16]. The basic physical mechanisms through which this happens in the ocean are advection and diffusion.

Advection is associated with the flow of a fluid; it is the process by which a tracer is transported from one location to another, due to the velocity field of the fluid in motion. In the ocean, there is strong experimental evidence on how physical effects such as elongation, shear, strain and rotation affect tracers' patches such as chlorphyll-a and hence play a role in algae blooms [5]. Molecular diffusion is another mode of transport that is associated with the random motions of the molecules within a fluid; diffusion happens from regions of high concentration to low concentration according to Fick's law. A more substantial effect on diffusing tracers in the ocean however is turbulent diffusion by eddies. The following analogy explains why: dissolved sugar takes a very long time to diffuse in a cup of coffee, relying only on molecular agitation. With a spoon, one can create eddies that transport dissolved sugar throughout the cup in less than a second [12]. This "enhanced" transport effect is generally described by what is called eddy diffusivity or viscocity.

Ocean flow is known to be turbulent due to the excessive fluctuations in the velocity field; this flow is characterized by eddies that occur over a wide range of length and time scales. Large eddies transporting momentum are dissipated by kinetic energy into small eddies that mix the tracer until it is completely diffused [3]. The tracer experiences stretching and straining due to velocity fluctuations and this is known as stirring. The effect of stirring and mixing is described by a turbulent diffusivity coefficient which is much greater than the molecular diffusion described by Fick's law.

At the end of the nineteenth century, Reynolds explained how a fully developed flow can be changed from laminar to turbulent through a pipe by decomposing the velocity into mean and fluctuating components

$$u(\vec{x},t) = \bar{u}(\vec{x}) + u'(\vec{x},t)$$

where the time-averaged field $\bar{u}$ is space-dependent and where the fluctuations u' are space and time dependent. He assumed that the flow is homogeneous in time, that is the statistics of the flow is invariant under any shift in time and isotropic, that is being subject to no variations in the direction of the motion. Reynolds predicted a "Reynolds number" at which a laminar flow becomes unstable [15]. Since then, this decomposition of velocity has become a very powerful method to resolve the effects of turbulence.

To quantify the effect of turbulence on pollutant concentration, Reynolds decomposition can be applied to a homogeneous flow to obtain a locally time averaged advection diffusion equation that contains the effect of the fluctuations of the velocity and the concentration as $< u'C' >$. This model needs closure by relating the fluctuating parts to the average concentration gradient through an "effective diffusivity" in a manner analogous to Fick's law of molecular diffusion. Many theories to quantify eddy diffusivity were introduced, the first among which was due to Taylor. His method which was founded in 1920 was widely used and considered breakthrough in later works that focus on estimating eddy diffusivity. Through his studies, Taylor attempted to relate Lagrangian eddy diffusivity, assuming a homogeneous stationary flow, to the autocorrelation of the Lagrangian fluctuation velocity and showed that $\frac{1}{2}\frac{d[X^2]}{dt} = D$ where $[X^2]$ is the mean square displacement of the particles and D is defined as the dispersion coefficient $D = [u^2]\int_0^t R_\tau d\tau$ [6]. Later, the term 'apparent diffusivity' has been commonly used ([14], [2]) and introduced as $K_a = \frac{1}{2}\frac{d\sigma^2}{dt}$ where the variance σ^2 is well defined and computed from either a radial symmetric distribution or a probability density function. Taylor [6] employed the concept of motion of air in his Lagrangian approach to diffusion by continuous movements. The deterministic approach to turbulence via the Navier Stokes equations of motion leads to the classical closure problem. Taylor [17], Prandtl [9] and von Karman [18] suggested semi empirical closure approximations to circumvent this problem. This approach to closure is based on the analogy between turbulence and molecular diffusion, leading to eddy diffusivity. Although the variety of scales in turbulence was recognized by Prandtl, he suggested that a simplification was possible by taking an average scale which is the mixing length. Mixing length forms the basis of many local closure models, including eddy diffusivity models.

In this thesis, we are interested in the advection diffusion equation for the mean concentration $C(\vec{x},t)$ of a tracer advected by a turbulent flow in which separation of scales in the manner treated by Prandtl is possible:

$$C_t + \vec{U}\cdot\nabla C = A\Delta C$$

,

where $\vec{U}$ is the mean flow due to large eddies and A is the effective diffusivity.

A physical based model of advection diffusion in two dimensions that takes into account the combined effect of diffusion due to small eddies, and differential advection due to large eddies was developed in the seminal work of Okubo [2]. The main contribution of this thesis is to extend this model to three dimensions. Specifically, we present an analytical solution to the advection diffusion equation in a three dimensional turbulent flow that captures essential physical effects such as rotation, deformation and shear. The equation governs the mean concentration of a tracer being advected, with a non-divergent mean flow being linear in space. The solution is based on transforming the Eulerian equation into a system of ordinary differential equations that descibe the trajectories and a diffusion equation in the Lagrangian frame, solving it with Fourier transform transforming it back to the Eulerian form. The contours of the solution are a set of ellipsoids with principal axes changing with time according to the linear flow parametersband to the diffusivity of the small eddies. We compute an apparent coefficient of diffusion that combines the effects of the advection with that of the turbulent diffusion. We illustrate our solution with simple linear flows that captures the basic deformation (rotation, stretching and shearing).

Solutions to the advection diffusion problem with a general mean velocity field can be obtained numerically. Eulerian and mesh dependent schemes such as finite difference methods (FDM), finite volume methods (FVM) and finite elements method (FEM) are all well established in the computation of multi-dimensional advection-diffusion problems. For a high Péclet number however, they suffer from nonphysical oscillations and excessive numerical diffusion [10]. Extreme mesh refinement may be one possible solution but it requires excessive computational requirements. Alternative formulations such as Lagrangian methods ([1], [8], [7]) are sought. Lagrangian methods advect particles along their trajectories according to the local velocity. We foresee that this solution can be employed in this context, where instead of the local uniform velocity, a linear one can be used.

The thesis is organized as follows. In chapter 2, we present the derivation of the advection diffusion equation in a three dimensional turbulent flow in which the mean flow is linear in space. In chapter 3, we present the derivation of the fundamental solution in three dimensions turbulent flow from which an apparent diffusion of coefficient that shows the combined effects of the advection and diffusion is inferred, and we explore the small and large asymptotic time behaviors of this coefficient. In chapter 4, we illustrate the solution and the apparent diffusivity for simple linear flows. In chapter 5, we present a paper titled "A fundamental solution for an advection diffusion equation in a non uniform three dimensional flow". In chapter 6, we state the conclusion and perspectives.

Chapter two
Governing equation for the concentration of a tracer in a turbulent flow with linear mean

In this chapter we provide the mathematical background to our equation of interest by reviewing the derivation of the advection diffusion equation in a turbulent flow, under the assumption of separation of scales using Reynolds decomposition. We also explain how to get the non isotropic case from the isotropic one.

2.1 Separation of scales in the velocity

A turbulent flow is characterized by high levels of fluctuating velocities populated by many eddies with different sizes that break down into smaller eddies until the energy is dissipated into heat.

Reynolds described how flow can change from laminar to turbulent by decomposing the velocity field into a statistical average $\bar{u}$ and a fluctuation component u'

$$u(x,y,z,t) = \bar{u}(x,y,z,t) + u'(x,y,z,t)$$

where

$$u(x,y,z,t) = \begin{bmatrix} U(x,y,z,t) \\ V(x,y,z,t) \\ W(x,y,z,t) \end{bmatrix}$$

and

$$\bar{u} = \frac{1}{T_I}\int_t^{t+T_I} u\, d\tau$$

where T_I is the integral time scale for the unresolved scale part u'. The resolved scale part $\overline{u}$ is defined over an Eulerian time scale T_E.

By using Reynolds decomposition analogy for the concentration of a tracer

$$C(x,y,z,t) = \bar{C}(x,y,z,t) + C'(x,y,z,t)$$

a new advection diffusion equation is derived with a turbulent diffusion coefficient greater than the molecular coefficient. The turbulent diffusion coefficient is the result of the fluctuation parts of the velocity and the average concentration of the tracer [11].

Considering the advection diffusion equation

$$\frac{\partial C}{\partial t} + \vec{u} \cdot \nabla C = D_m \Delta C,$$

where

$$C = \bar{C} + C',$$
$$u = \bar{u} + u',$$

and D_m is the molecular diffusion coefficient.

By taking the time average over the integral time scale T_I, the advection diffusion equation becomes

$$\frac{\partial \bar{C}}{\partial t} + \overline{\vec{u}} \cdot \nabla C = -\nabla(\overline{u'C'}) + D_m \Delta C.$$

Since $u'C'$ is a flux term and using Fick's law type relation, we close this model by relating the time average turbulent flux to the gradient of the average concentration (mixing length theory)

$$\overline{u'C'} = A \nabla \bar{C},$$

where A is an effective diffusivity coefficient that is much greater than the molecular diffusion coefficient D_m .

The approach in defining the effective diffusivity is analogous to Prandtl's mixing length theory [9] since the characteristic time and length scales for the small scale eddies responsible for internal mixing due to the fluctuations in the velocity field are very small.

2.2 Governing equation for the concentration in a turbulent flow with linear mean

We represent the three dimensional advection diffusion equation in a turbulent isotropic flow. Using the assumption of the scale of separation, the large-scale eddies providing the inhomogeneity in the mean velocity field $\vec{u} = (U, V, W)$ and the small-scale eddies responsible for internal mixing due to fluctuation in the velocity field are separated by a length scale where the diffusion lies in between.

The advection diffusion equation is given by

$$\begin{aligned}&\frac{\partial S}{\partial t} + U(x,y,z)\frac{\partial S}{\partial x} + V(x,y,z)\frac{\partial S}{\partial y} + W(x,y,z)\frac{\partial S}{\partial z} \\ &= A\left(\frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2} + \frac{\partial^2 S}{\partial z^2}\right),\end{aligned} \tag{2.1}$$

where S is the concentration of the tracer. The velocity field is averaged over a time scale that is much less than the Eulerian time scale T_E so that we can assume the mean flow $\vec{U}$ is only space-dependent. The eddy diffuisivity A is assumed to be constant in space and time since the characteristic time of the small scale eddies are very small compared to the observation time scale.

Assuming the mean flow is linear, $\vec{u}$ is approximated by linear fuctions using Taylor expansion around the center of the patch (x_0, y_0, z_0). The governing equation can be rewritten, in the moving reference frame, as follows

$$\begin{aligned}&S_t + \left[\left(\frac{\partial U}{\partial x}\right)_0 x + \left(\frac{\partial U}{\partial y}\right)_0 y + \left(\frac{\partial U}{\partial z}\right)_0 z\right] S_x \\ &\left[\left(\frac{\partial V}{\partial x}\right)_0 x + \left(\frac{\partial V}{\partial y}\right)_0 y + \left(\frac{\partial V}{\partial z}\right)_0 z\right] S_y \\ &\left[\left(\frac{\partial W}{\partial x}\right)_0 x + \left(\frac{\partial W}{\partial y}\right)_0 y + \left(\frac{\partial W}{\partial z}\right)_0 z\right] S_z \\ &= A\,\Delta S,\end{aligned} \tag{2.2}$$

where the Laplacian is $\Delta S \equiv S_{xx} + S_{yy} + S_{zz}$ and where the zero script indicates that the velocity gradients are evaluated at the center of the patch.

Denoting by

$$\alpha = \left(\frac{\partial U}{\partial x}\right)_0, \quad \beta = \left(\frac{\partial V}{\partial y}\right)_0, \quad \gamma = \left(\frac{\partial W}{\partial z}\right)_0 \text{ : stretching deformation} \tag{2.3}$$

$$\vec{h} = \begin{bmatrix} h_{xy} = \frac{1}{2}(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y})_0 \\ h_{xz} = \frac{1}{2}\frac{\partial u}{\partial z} \\ h_{yz} = \frac{1}{2}\frac{\partial v}{\partial z} \end{bmatrix} \text{ : shearing deformation} \tag{2.4}$$

$$\vec{\eta} = \begin{bmatrix} \eta_{xy} = \frac{1}{2}(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y})_0 \\ \eta_{xz} = \frac{1}{2}\frac{\partial u}{\partial z} \\ \eta_{yz} = -\frac{1}{2}\frac{\partial v}{\partial z} \end{bmatrix} \text{ : vorticity} \tag{2.5}$$

and assuming the non divergence in the mean velocity field, $\gamma = -\alpha - \beta$, with the vertical velocity component with respect to x and y are negligible $\frac{\partial W}{\partial x} = \frac{\partial W}{\partial y} = 0$, the three dimensional advection diffusion equation is then

$$S_t + \Big(\alpha x + (h_{xy} - \eta_{xy})y + (h_{xz} + \eta_{xz})z\Big)S_x + \Big((h_{xy} - \eta_{xy})x + \beta y + (h_{yz} - \eta_{yz})z\Big)S_y + \gamma z S_z = A\,\Delta S \tag{2.6}$$

subject to the initial condition the initial condition the delta function in space with strength Q

$$S(0,x,y,z) = Q\,\delta(x)\delta(y)\delta(z)$$

In case of a non isotropic flow, a new eddy diffusivity B in the z-direction is considered. Eq. (2.2) becomes

$$\begin{aligned} & S_t + \left[\left(\frac{\partial U}{\partial x}\right)_0 x + \left(\frac{\partial U}{\partial y}\right)_0 y + \left(\frac{\partial U}{\partial z}\right)_0 z\right] S_x \\ & \left[\left(\frac{\partial V}{\partial x}\right)_0 x + \left(\frac{\partial V}{\partial y}\right)_0 y + \left(\frac{\partial V}{\partial z}\right)_0 z\right] S_y \\ & \left[\left(\frac{\partial W}{\partial x}\right)_0 x + \left(\frac{\partial W}{\partial y}\right)_0 y + \left(\frac{\partial W}{\partial z}\right)_0 z\right] S_z \\ & = A(S_{xx} + S_{yy}) + B S_{zz}, \end{aligned} \tag{2.7}$$

such that

$$S(0,x,y,z) = Q\,\delta(x)\delta(y)\delta(z).$$

Taking $z^* = \sqrt{A/B}z$, and $W^* = \sqrt{A/B}w$ yields

$$\begin{aligned}
&S_t + \left[\left(\frac{\partial U}{\partial x}\right)_0 x + \left(\frac{\partial U}{\partial y}\right)_0 y + \left(\frac{\partial U}{\partial z^*}\right)_0 z^*\right] S_x \\
&\left[\left(\frac{\partial V}{\partial x}\right)_0 x + \left(\frac{\partial V}{\partial y}\right)_0 y + \left(\frac{\partial V}{\partial z^*}\right)_0 z^*\right] S_y \\
&\left[\left(\frac{\partial W^*}{\partial x}\right)_0 x + \left(\frac{\partial W^*}{\partial y}\right)_0 y + \left(\frac{\partial W^*}{\partial z^*}\right)_0 z^*\right] S_{z^*} \\
&= A\left(S_{xx} + S_{yy} + S_{z^*z^*}\right) \qquad (2.8)
\end{aligned}$$

such that

$$S(0, x, y, z) = \sqrt{A/B}\, Q\, \delta(x)\, \delta(y)\, \delta(z).$$

The solution methodology remains the same after rescaling.

Chapter Three

Derivation of the fundamental solution for the concentration in a turbulent flow with linear mean

We aim to solve equation (2.6). For this purpose, we represent the concentration $S(t,x,y,z)$ in the Lagrangian frame of reference

$$\Gamma(t,a,b,c) \equiv S(t,x(a,b,c),y(t,a,b,c),z(a,b,c)) \tag{3.1}$$

where a, b and c represent the initial coordinates of a substance, and $x(t,a,b,c)$, $y(t,a,b,c)$ and $z(t,a,b,c)$ are its coordinates at t.

Proposition 1. *Equation (2.6) can be tranformed into the following ODE system for the displacements and the Lagrangian diffusion equation:*

$$\frac{d}{dt}\begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} = \mathbf{T}\begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix}, \tag{3.2}$$

$$\Gamma_t = A\Big([[\Gamma,y,z],y,z] + [x,[x,\Gamma,z],z] + [x,y,[x,y,\Gamma]]\Big), \tag{3.3}$$

where

$$\mathbf{T} = \begin{bmatrix} \alpha & h_{xy}-\eta_{xy} & h_{xz}+\eta_{xz} \\ h_{xy}+\eta_{xy} & \beta & h_{yz}-\eta_{yz} \\ 0 & 0 & \gamma \end{bmatrix}$$

, and the bracket notation stands for the Jacobian, i.e. $[A,B,C] = \dfrac{\partial(A,B,C)}{\partial(a,b,c)}$.

Proof. Using (3.1) and the chain rule, we see that

$$\Gamma_t = \frac{DS}{Dt} = S_t + S_x x_t + S_y y_t + S_z z_t \tag{3.4}$$

and using (3.2) and (2.6), we see that

$$\begin{aligned} \Gamma_t = \frac{DS}{Dt} &= S_t + \mathbf{T}\begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} \cdot \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} \\ &= A\Delta S. \end{aligned} \tag{3.5}$$

By expressing the partial derivatives of S in terms of those of Γ using the chain rule again

$$
\begin{aligned}
S_{xx} &= [[\Gamma, y, z], y, z],\\
S_{yy} &= [x, [x, \Gamma, z], z],\\
S_{zz} &= [x, y, [x, y, \Gamma]],
\end{aligned}
\tag{3.6}
$$

the result follows.

$\square$

3.1 Solution of the concentration in the Lagrangian frame

We solve (3.3) by diagonalizing the ODE system (3.2). The eigenvalues are found to be

$$
\begin{aligned}
\lambda_1 &= -\alpha-\beta,\\
\lambda_2 &= \frac{1}{2}\left[(\alpha+\beta)+\left((\alpha-\beta)^2+4(h_{xy}^2-\eta_{xy}^2)\right)^{1/2}\right],\\
\lambda_3 &= \frac{1}{2}\left[(\alpha+\beta)-\left((\alpha-\beta)^2+4(h_{xy}^2-\eta_{xy}^2)\right)^{1/2}\right],
\end{aligned}
\tag{3.7}
$$

with their corresponding eigenvectors

$$
\vec{V_1} = \begin{bmatrix} \frac{(\alpha+2\beta)(h_{xz}+\eta_{xz})-(h_{xy}-\eta_{xy})(h_{yz}-\eta_{yz})}{-2\alpha^2-2\beta^2-5\alpha\beta+h_{xy}^2-\eta_{xy}^2} \\ \frac{(2\alpha+\beta)(h_{yz}-\eta_{yz})-(h_{xy}+\eta_{xy})(h_{xz}+\eta_{xz})}{-2\alpha^2-2\beta^2-5\alpha\beta+h_{xy}^2-\eta_{xy}^2} \\ 1 \end{bmatrix},
$$

$$
\vec{V_2} = \begin{bmatrix} \frac{\alpha-\beta+\left((\alpha-\beta)^2+4(h_{xy}^2-\eta_{xy}^2)\right)^{1/2}}{2(h_{xy}+\eta_{xy})} \\ 1 \\ 0 \end{bmatrix},
$$

$$
\vec{V_3} = \begin{bmatrix} \frac{\alpha-\beta-\left((\alpha-\beta)^2+4(h_{xy}^2-\eta_{xy}^2)\right)^{1/2}}{2(h_{xy}+\eta_{xy})} \\ 1 \\ 0 \end{bmatrix}.
$$

The Lagrangian displacements are obtained in terms of a, b and c

$$
\begin{aligned}
x(t;a,b,c) &= a\,e^{\frac{(\alpha+\beta)t}{2}}\left(\cosh\frac{\sqrt{M}t}{2}+\frac{\alpha-\beta}{\sqrt{M}}\sinh\frac{\sqrt{M}t}{2}\right)+\frac{2b}{\sqrt{M}}(h_{xy}-\eta_{xy})e^{\frac{(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2}\\
&\quad+\frac{c}{S}\left[P\left(e^{\frac{(\alpha+\beta)t}{2}}\cosh\frac{\sqrt{M}}{2}t-e^{-(\alpha+\beta)t}\right)+e^{\frac{(\alpha+\beta)}{2}t}\frac{Q}{\sqrt{M}}\sinh\frac{\sqrt{M}}{2}t\right], \qquad (3.8)\\
y(t;a,b,c) &= b\,e^{\frac{(\alpha+\beta)t}{2}}\left(\cosh\frac{\sqrt{M}t}{2}-\frac{\alpha-\beta}{\sqrt{M}}\sinh\frac{\sqrt{M}t}{2}\right)+\frac{2a}{\sqrt{M}}(h_{xy}+\eta_{xy})e^{\frac{(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2}\\
&\quad+\frac{c}{S}\left[P'\left(e^{\frac{(\alpha+\beta)t}{2}}\cosh\frac{\sqrt{M}}{2}t-e^{-(\alpha+\beta)t}\right)+e^{\frac{(\alpha+\beta)}{2}t}\frac{Q'}{\sqrt{M}}\sinh\frac{\sqrt{M}}{2}t\right], \qquad (3.9)\\
z(t;a,b,c) &= c\,e^{-(\alpha+\beta)t}, \qquad (3.10)
\end{aligned}
$$

where

$$
\begin{aligned}
M &= (\alpha-\beta)^2+4(h_{xy}^2-\eta_{xy}^2),\\
S &= -2(\alpha^2+\beta^2)-5\alpha\beta+(h_{xy}^2-\eta_{xy}^2),\\
P &= (h_{xy}-\eta_{xy})(h_{yz}-\eta_{yz})-(h_{xz}+\eta_{xz})(\alpha+2\beta),\\
Q &= 2(h_{xy}-\eta_{xy})P'+(\alpha-\beta)P, \qquad (3.11)\\
P' &= (h_{xy}+\eta_{xy})(h_{xz}+\eta_{xz})-(h_{yz}-\eta_{yz})(2\alpha+\beta),\\
Q' &= 2(h_{xy}+\eta_{xy})P-(\alpha-\beta)P'.
\end{aligned}
$$

Note that if $M=0$, we replace, at this stage, $\dfrac{\sinh\sqrt{M}t/2}{\sqrt{M}}$ by $t/2$. Otherwise, we may assume $M\neq 0$

Now the right hand side of (3.3) can be simplified

$$
\begin{aligned}
[[\Gamma,y,z],y,z] &= \Gamma_{aa}(y_bz_c)^2+\Gamma_{bb}(y_az_c)^2-2\Gamma_{ab}y_ay_bz_c^2,\\
[x,[x,\Gamma,z],y,z] &= \Gamma_{aa}(x_bz_c)^2+\Gamma_{bb}(x_az_c)^2-2\Gamma_{ab}x_ax_bz_c^2,\\
[x,y,[x,y,\Gamma]] &= \Gamma_{aa}(x_by_c-x_cy_b)^2+\Gamma_{bb}(x_ay_c-x_cy_a)^2+\Gamma_{cc}(x_ay_b-x_by_a)^2\\
&\quad-2\Gamma_{ab}\left(x_c^2y_ay_b+y_c^2x_ax_b-x_ax_cy_by_c-x_bx_cy_ay_c\right)\\
&\quad-2\Gamma_{ac}\left(x_b^2y_ay_c+y_b^2x_ax_c-x_ax_by_by_c-x_bx_cy_ay_b\right)\\
&\quad-2\Gamma_{bc}\left(x_a^2y_by_c+y_a^2x_bx_c-x_ax_cy_ay_b-x_ax_by_ay_c\right).
\end{aligned}
$$

The diffusion equation for Γ is now

$$\frac{\partial \Gamma}{\partial t} = A\Big(F_1(t)\frac{\partial^2\Gamma}{\partial a^2} + F_2(t)\frac{\partial^2\Gamma}{\partial b^2} + F_3(t)\frac{\partial^2\Gamma}{\partial c^2} - 2G_1(t)\frac{\partial^2\Gamma}{\partial a\partial b} - 2G_2(t)\frac{\partial^2\Gamma}{\partial a\partial c} - 2G_3(t)\frac{\partial^2\Gamma}{\partial b\partial c}\Big) \tag{3.12}$$

where the time dependent coefficients on the right hand side are given by

$$\begin{aligned}
F_1(t) &= z_c^2(x_b^2+y_b^2) + (x_c y_b - x_b y_c)^2,\\
F_2(t) &= z_c^2(x_a^2+y_a^2) + (x_a y_c - x_c y_a)^2,\\
F_3(t) &= (x_a y_b - x_b y_a)^2,\\
G_1(t) &= z_c^2(x_a x_b + y_a y_b) - (x_a y_c - x_c y_a)(x_c y_b - x_b y_c),\\
G_2(t) &= (x_a y_b - x_b y_a)(x_c y_b - x_b y_c),\\
G_3(t) &= (x_a y_b - x_b y_a)(x_a y_c - x_c y_a).
\end{aligned} \tag{3.13}$$

Equation (3.12) is solved using Fourier transform

$$\hat{\Gamma}(t,w_1,w_2,w_3) = \frac{1}{8\pi^3}\int\int\int \Gamma(t,a,b,c)e^{-iw_1a-iw_2b-iw_3c}\,da\,db\,dc. \tag{3.14}$$

Thus, the equation governing the Fourier transform of Γ is

$$\hat{\Gamma}_t = A\hat{\Gamma}\Big(-w_1^2F_1 - w_2^2F_2 - w_3^2F_3 + 2w_1w_2G_1 + 2w_1w_3G_2 + 2w_2w_3G_3\Big), \tag{3.15}$$

with solution

$$\hat{\Gamma}(t;w_1,w_2,w_3) = e^{-A\int_0^t \Big(F_1w_1^2 + F_2w_2^2 + F_3w_3^2 - 2w_1w_2G_1 - 2w_1w_3G_2 - 2w_2w_3G_3\Big)d\tau} \times c(w_1,w_2,w_3), \tag{3.16}$$

where

$$c(w_1,w_2,w_3) = \frac{Q}{8\pi^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(a)\,\delta(b)\,\delta(c)\,e^{iw_1a}\,e^{iw_2b}\,e^{iw_3c}\,da\,db\,dc. \tag{3.17}$$

The solution of the concentration in the Lagrangian frame is

$$\Gamma(t,a,b,c) = \frac{Q}{8(A\pi)^{3/2}R}\times \tag{3.18}$$
$$e^{-\frac{1}{4AR^2}\big(a^2(\overline{F}_2\overline{F}_3-\overline{G}_3^2)+b^2(\overline{F}_1\overline{F}_3-\overline{G}_2^2)+c^2(\overline{F}_1\overline{F}_2-\overline{G}_1^2)+2ab(\overline{G}_2\overline{G}_3+\overline{G}_1\overline{F}_3)+2ac(\overline{G}_1\overline{G}_3+\overline{G}_2\overline{F}_2)+2bc(\overline{G}_1\overline{G}_2+\overline{G}_3\overline{F}_1)\big)},$$

where

$$
\begin{aligned}
\overline{F_1}(t) &= \int_0^t F_1(\tau)\,d\tau \qquad (3.19)\\
&= \left\{\frac{A}{M(M-\gamma^2)} - \frac{\gamma(Q^2+MP^2)+2MPQ}{2M(M-\gamma^2)S^2}\right\}e^{\gamma t}\cosh\sqrt{M}t\\
&+ \left\{\frac{A'}{\sqrt{M}(M-\gamma^2)} + \frac{(Q^2+MP^2)+2\gamma PQ}{2\sqrt{M}(M-\gamma^2)S^2}\right\}e^{\gamma t}\sinh\sqrt{M}t\\
&+ \left\{\frac{4PQ-4\gamma P^2}{(M-\gamma^2)S^2}\right\}e^{\frac{-\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + \left\{\frac{4\gamma PQ-4MP^2}{\sqrt{M}(M-\gamma^2)S^2}\right\}e^{\frac{-\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}\\
&+ \left\{\frac{4\eta_{xy}(h_{xy}-\eta_{xy})}{\gamma M} - \frac{Q^2-MP^2}{2\gamma S^2 M}\right\}e^{\gamma t} - \frac{P^2}{2\gamma S^2}e^{-2\gamma t}\\
&+ \left\{\frac{A''}{\gamma M(M-\gamma^2)} + \frac{Q^2+9\gamma^2P^2-6\gamma PQ}{2\gamma(M-\gamma^2)S^2}\right\}\\
\overline{F_2}(t) &= \int_0^t F_2(\tau)\,d\tau\\
&= \left\{\frac{B}{M(M-\gamma^2)} - \frac{\gamma(Q'^2+MP'^2)+2MP'Q'}{2M(M-\gamma^2)S^2}\right\}e^{\gamma t}\cosh\sqrt{M}t\\
&+ \left\{\frac{B'}{\sqrt{M}(M-\gamma^2)} + \frac{(Q'^2+MP'^2)+2\gamma P'Q'}{2\sqrt{M}(M-\gamma^2)S^2}\right\}e^{\gamma t}\sinh\sqrt{M}t\\
&+ \left\{\frac{4P'Q'-4\gamma P'^2}{(M-\gamma^2)S^2}\right\}e^{\frac{-\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + \left\{\frac{4\gamma P'Q'-4MP'^2}{\sqrt{M}(M-\gamma^2)S^2}\right\}e^{\frac{-\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}\\
&+ \left\{\frac{-4\eta_{xy}(h_{xy}+\eta_{xy})}{\gamma M} - \frac{Q'^2-MP'^2}{2\gamma S^2 M}\right\}e^{\gamma t} - \frac{P'^2}{2\gamma S^2}e^{-2\gamma t}\\
&+ \left\{\frac{B''}{\gamma M(M-\gamma^2)} + \frac{Q'^2+9\gamma^2P'^2-6\gamma P'Q'}{2\gamma(M-\gamma^2)S^2}\right\}\\
\overline{F_3}(t) &= \int_0^t F_3(\tau)\,d\tau\\
&= -\frac{e^{-2\gamma t}}{2\gamma}
\end{aligned}
$$

$$
\begin{aligned}
\overline{G_1}(t) &= \int_0^t G_1(\tau)\,d\tau \\
&= \left\{\frac{C}{M(M-\gamma^2)} + \frac{\gamma(QQ'+PP'M)+(P'Q+PQ')M}{2S^2M(M-\gamma^2)}\right\}e^{\gamma t}\cosh\sqrt{M}t \\
&+ \left\{\frac{C'}{\sqrt{M}(M-\gamma^2)} - \frac{(QQ'+MPP')+\gamma(PQ'+P'Q)}{2S^2\sqrt{M}(M-\gamma^2)}\right\}e^{\gamma t}\sinh\sqrt{M}t \\
&+ \left\{\frac{4\gamma PP'-2(PQ'+P'Q)}{S^2(M-\gamma^2)}\right\}e^{\frac{-\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} \\
&+ \left\{\frac{4MPP'-2\gamma(PQ'+P'Q)}{S^2\sqrt{M}(M-\gamma^2)}\right\}e^{\frac{-\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2} \\
&+ \left\{\frac{2\eta_{xy}(\alpha-\beta)}{\gamma M} + \frac{QQ'-MPP'}{2\gamma MS^2}\right\}e^{\gamma t} + \frac{PP'}{2\gamma S^2}e^{-2\gamma t} \\
&+ \left\{\frac{MC''}{\gamma M(M-\gamma^2)} - \frac{QQ'+9\gamma^2PP'-3\gamma(PQ'+P'Q)}{2\gamma(M-\gamma^2)S^2}\right\} \\
\overline{G_2}(t) &= \int_0^t G_2(\tau)\,d\tau \\
&= \frac{2(Q-\gamma P)}{(M-\gamma^2)S}e^{\frac{-\gamma}{2}t}\cosh\frac{\sqrt{M}t}{2} + \frac{2(\gamma Q-PM)}{\sqrt{M}(M-\gamma^2)S}e^{\frac{-\gamma}{2}t}\sinh\frac{\sqrt{M}t}{2} - \frac{P}{2\gamma S}e^{-2\gamma t} + \frac{(M+3\gamma^2)P-4\gamma Q}{2\gamma(M-\gamma^2)S} \\
\overline{G_3}(t) &= \int_0^t G_3(\tau)\,d\tau \\
&= \frac{2(Q'-\gamma P')}{(M-\gamma^2)S}e^{\frac{-\gamma}{2}t}\cosh\frac{\sqrt{M}t}{2} + \frac{2(\gamma Q'-P'M)}{\sqrt{M}(M-\gamma^2)S}e^{\frac{-\gamma}{2}t}\sinh\frac{\sqrt{M}t}{2} - \frac{P'}{2\gamma S}e^{-2\gamma t} + \frac{(M+3\gamma^2)P'-4\gamma Q'}{2\gamma(M-\gamma^2)S}
\end{aligned}
\tag{3.20}
$$

and

$$
\begin{aligned}
A &= 2\beta(\alpha-\beta)^2 + 4h_{xy}(h_{xy}-\eta_{xy})(\alpha+\beta) - 4(h_{xy}^2-\eta_{xy}^2)(\alpha-\beta), \\
A' &= -2\beta(\alpha-\beta) + 4h_{xy}(h_{xy}-\eta_{xy}), \\
A'' &= -\gamma A - 4\eta_{xy}(h_{xy}-\eta_{xy})(M-\gamma^2), \\
B &= 2\alpha(\alpha-\beta)^2 + 4h_{xy}(h_{xy}+\eta_{xy})(\alpha+\beta) + 4(h_{xy}^2-\eta_{xy}^2)(\alpha-\beta), \\
B' &= 2\alpha(\alpha-\beta) + 4h_{xy}(h_{xy}+\eta_{xy}), \\
B'' &= -\gamma B + 4\eta_{xy}(h_{xy}+\eta_{xy})(M-\gamma^2), \\
C &= 2h_{xy}(\alpha-\beta)^2 + 8h_{xy}(h_{xy}^2-\eta_{xy}^2) - 2\eta_{xy}(\alpha^2-\beta^2), \\
C' &= 2h_{xy}(\alpha+\beta) - 2\eta_{xy}(\alpha-\beta), \\
C'' &= 2h_{xy}(\alpha+\beta) - 2\eta_{xy}(\alpha-\beta),
\end{aligned}
\tag{3.21}
$$

and

$$R(t) = \left\{\overline{F}_3(\overline{F}_1\overline{F}_2 - \overline{G}_1^2) - \overline{G}_3(\overline{G}_1\overline{G}_2 + \overline{G}_3\overline{F}_1) - \overline{G}_2(\overline{G}_1\overline{G}_3 + \overline{G}_2\overline{F}_2)\right\}^{1/2}. \tag{3.22}$$

3.2 Solution of the concentration in the Eulerian frame

The Lagrangian solution is transformed back to its Eulerian form by obtaining a, b and c in terms of x, y and z

$$\begin{aligned}
a &= xe^{-\frac{(\alpha+\beta)t}{2}}\left(\cosh\frac{\sqrt{M}t}{2} - \frac{(\alpha-\beta)}{\sqrt{M}}\sinh\frac{\sqrt{M}t}{2}\right) - \frac{2y(h_{xy}-\eta_{xy})}{\sqrt{M}}e^{-\frac{(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2} \\
&+ z\left[\frac{P}{S}\left(e^{\frac{-(\alpha+\beta)t}{2}}\cosh\frac{\sqrt{M}t}{2} - e^{(\alpha+\beta)t}\right) - \frac{Q}{S\sqrt{M}}e^{\frac{-(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2}\right], \\
b &= ye^{-\frac{(\alpha+\beta)t}{2}}\left(\cosh\frac{\sqrt{M}t}{2} + \frac{(\alpha-\beta)}{\sqrt{M}}\sinh\frac{\sqrt{M}t}{2}\right) - \frac{2x(h_{xy}+\eta_{xy})}{\sqrt{M}}e^{-\frac{(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2} \\
&+ z\left[\frac{P'}{S}\left(e^{\frac{-(\alpha+\beta)t}{2}}\cosh\frac{\sqrt{M}t}{2} - e^{(\alpha+\beta)t}\right) - \frac{Q'}{S\sqrt{M}}e^{\frac{-(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2}\right], \\
c &= ze^{(\alpha+\beta)t},
\end{aligned}$$

and substituting them in (2.6).

The Eulerian solution is a Gaussian of the form

$$S(t,x,y,z) = \frac{Q}{8(A\pi)^{3/2}R(t)}e^{-\frac{C_{x^2}(t)x^2 + C_{y^2}(t)y^2 + C_{z^2}(t)z^2 + C_{xy}(t)xy + C_{xz}(t)xz + C_{yz}(t)yz}{4AR^2(t)}} \tag{3.23}$$

along with coefficients defined as

$$
\begin{aligned}
C_{x^2}(t) &= C_x^1(\alpha,\beta,\vec{h},\vec{\eta}) + C_x^2(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} + C_x^3(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{\gamma t}{2}} \cosh \frac{\sqrt{M}t}{2} \\
&+ C_x^4(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{\gamma t}{2}} \sinh \frac{\sqrt{M}t}{2}}{\sqrt{M}} + C_x^5(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \cosh \sqrt{M}t \\
&+ C_x^6(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\gamma t} \sinh \sqrt{M}t}{\sqrt{M}} + C_x^7(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} \cosh \sqrt{M}t \\
&+ C_x^8(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{-\gamma t} \sinh \sqrt{M}t}{\sqrt{M}} + C_x^9(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} \\
&+ C_x^{10}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{2\gamma t}, \\
C_{y^2}(t) &= C_y^1(\alpha,\beta,\vec{h},\vec{\eta}) + C_y^2(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} + C_y^3(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{\gamma t}{2}} \cosh \frac{\sqrt{M}t}{2} \\
&+ C_y^4(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{\gamma t}{2}} \sinh \frac{\sqrt{M}t}{2}}{\sqrt{M}} + C_x^5(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \cosh \sqrt{M}t \\
53 &+ C_y^6(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\gamma t} \sinh \sqrt{M}t}{\sqrt{M}} + C_y^7(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} \cosh \sqrt{M}t \\
&+ C_y^8(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{-\gamma t} \sinh \sqrt{M}t}{\sqrt{M}} + C_y^9(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} \\
&+ C_y^{10}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{2\gamma t}, \\
C_{z^2}(t) &= C_z^1(\alpha,\beta,\vec{h},\vec{\eta}) + C_z^2(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \\
&+ C_z^3(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{\gamma t}{2}} \cosh \frac{\sqrt{M}t}{2} + C_z^4(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{\gamma t}{2}} \sinh \frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
&+ C_z^5(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \cosh \sqrt{M}t + C_z^6(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\gamma t} \sinh \sqrt{M}t}{\sqrt{M}} \\
&+ C_z^7(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} \cosh \sqrt{M}t + C_z^8(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{-\gamma t} \sinh \sqrt{M}t}{\sqrt{M}} \\
&+ C_z^9(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{-\gamma t}{2}} \cosh \frac{\sqrt{M}t}{2} + C_z^{10}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{-\gamma t}{2}} \sinh \frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
&+ C_z^{11}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} + C_z^{12}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-2\gamma t} + C_z^{13}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{2\gamma t},
\end{aligned}
$$

$$
\begin{aligned}
C_{xy}(t) = {} & C^1_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) + C^2_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \\
& + C^3_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{\gamma t}{2}} \cosh\frac{\sqrt{M}t}{2} + C^4_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{\gamma t}{2}} \sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^5_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \cosh\sqrt{M}t + C^6_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\gamma t} \sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^7_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} \cosh\sqrt{M}t + C^8_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{-\gamma t} \sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^9_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} + C^{10}_{xy}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{2\gamma t},
\end{aligned}
$$

$$
\begin{aligned}
C_{yz}(t) = {} & C^1_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) + C^2_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \\
& + C^3_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{\gamma t}{2}} \cosh\frac{\sqrt{M}t}{2} + C^4_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{\gamma t}{2}} \sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^5_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \cosh\sqrt{M}t + C^6_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\gamma t} \sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^7_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} \cosh\sqrt{M}t + C^8_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{-\gamma t} \sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^9_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{-\gamma t}{2}} \cosh\frac{\sqrt{M}t}{2} + C^{10}_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{-\gamma t}{2}} \sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^{11}_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} + C^{12}_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{2\gamma t}, \\
C_{xz}(t) = {} & C^1_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) + C^2_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \\
& + C^3_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{\gamma t}{2}} \cosh\frac{\sqrt{M}t}{2} + C^4_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{\gamma t}{2}} \sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^5_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\gamma t} \cosh\sqrt{M}t + C^6_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\gamma t} \sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^7_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} \cosh\sqrt{M}t + C^8_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{-\gamma t} \sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^9_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{\frac{-\gamma t}{2}} \cosh\frac{\sqrt{M}t}{2} + C^{10}_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, \frac{e^{\frac{-\gamma t}{2}} \sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^{11}_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{-\gamma t} + C^{12}_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\, e^{2\gamma t} \qquad (3.24)
\end{aligned}
$$

and

$$
\begin{aligned}
R^2(t) = & R_1(\alpha,\beta,\vec{h},\vec{\eta}) \cosh \frac{\sqrt{M}t}{2}\left(e^{\frac{\gamma t}{2}} - e^{\frac{-\gamma t}{2}}\right) \\
& + R_2(\alpha,\beta,\vec{h},\vec{\eta}) \cosh \sqrt{M}t\left(e^{\gamma t} - e^{-\gamma t}\right) \\
& + R_3(\alpha,\beta,\vec{h},\vec{\eta})\left(\frac{\sinh \sqrt{M}t}{\sqrt{M}}\left[e^{\gamma t} + e^{-\gamma t}\right] - \frac{2\sinh \frac{\sqrt{M}t}{2}}{\sqrt{M}}\left[e^{\frac{\gamma t}{2}} + e^{\frac{-\gamma t}{2}}\right]\right) \\
& + R_4(\alpha,\beta,\vec{h},\vec{\eta})\left(e^{\gamma t} - e^{-\gamma t}\right) \\
& + R_5(\alpha,\beta,\vec{h},\vec{\eta})\left(e^{2\gamma t} - e^{-2\gamma t}\right),
\end{aligned}
\tag{3.25}
$$

and where C_x^i (A.1), C_y^i (A.2), C_z^i (A.3), C_{xy}^i (A.4), C_{yz}^i (A.5) C_{xz}^i (A.6) and R_i (A.7) $(i = 1,..,13)$ are defined in the appendix.

3.3 Small time behavior of the solution

We study the small time behavior of the solution (3.23). The solution can be written as follows

$$
S(t,x,y,z) = \frac{Q}{8(A\pi)^{3/2}R(t)} e^{-\left(\frac{x^2}{\sigma^2_{x^2}(t)} + \frac{y^2}{\sigma^2_{y^2}(t)} + \frac{z^2}{\sigma^2_{z^2}(t)} + \frac{xy}{\sigma^2_{xy}(t)} + \frac{xz}{\sigma^2_{xz}(t)} + \frac{yz}{\sigma^2_{yz}(t)}\right)}. \tag{3.26}
$$

We expand the coefficients (3.24) and (3.25) of the solution in Taylor series around $t = 0$

$$
\begin{aligned}
\sigma^2_{x^2} = & \frac{4AR^2(t)}{C_{x^2}} \\
& \sim 4At + 4A\alpha t^2 + \\
& 4A\left[(2/3)\alpha^2 + (1/12)h_{xz}^2 - (1/3)h_{xy}^2 + (1/6)\eta_{xz}h_{xz} + (1/12)\eta_{xz}^2 - (2/3)h_{xy}\eta_{xy}\right]t^3 + O(t^4),
\end{aligned}
$$

$$
\begin{aligned}
\sigma^2_{y^2} = & \frac{4AR^2(t)}{C_{y^2}} \\
& \sim 4At + 4\beta At^2 + \\
& 4A\left[(2/3)\beta^2 + (1/12)h_{yz}^2 - (1/3)h_{xy}^2 + (1/6)\eta_{yz}h_{yz} + (1/12)\eta_{yz}^2 - (2/3)h_{xy}\eta_{xy}\right]t^3 + O(t^4),
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{z^2}^2 &= \frac{4AR^2(t)}{C_{z^2}} \\
&\sim 4At + 4A\gamma t^2 + \\
&4A\Big[(2/3)\alpha^2 + (2/3)\beta^2 + (4/3)\alpha\beta - (1/2)\eta_{xz} hxz + (1/2)\eta_{yz} hyz - (1/4)h_{xz}^2 - (1/4)h_{yz}^2 - (1/4)\eta_{xz}^2 \\
&- (1/4)\eta_{yz}^2\Big] t^3 + O(t^4),
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{xy}^2 &= \frac{4AR^2(t)}{C_x y} \\
&- \frac{2A}{h_{xy}} + \frac{A}{6\eta_{xy}^2}(h_{xz}h_{yz} - \eta_{yz}h_{xz} + \eta_{xz}h_{yz} - \eta_{xz}\eta_{yz} - 4h_{xy}\beta - 4\eta_{xy}\beta - 4h_{xy}\alpha + 4\eta_{xy}\alpha)t + O(t^2),
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{yz}^2 &= \frac{4AR^2(t)}{C_{yz}} \\
&\frac{4A}{\eta_{yz} - h_{yz}} + \frac{4A}{3(\eta_{yz} - h_{yz})^2}(-2h_{xy}h_{xz} - 2\eta_{xz}h_{xy} + \eta_{xy}h_{xz} + \eta_{xy}\eta_{xz} - 2h_{yz}\beta + 2\eta_{yz}\beta)t + O(t^2),
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{xz}^2 &= \frac{4AR^2(t)}{C_{xz}} \\
&- \frac{4A}{\eta_{xz} + h_{xz}} - \frac{4A}{3(\eta_{xz} + h_{xz})^2}(2h_{xy}h_{yz} - 2\eta_{yz}h_{xy} + \eta_{xy}h_{yz} - \eta_{xy}\eta_{yz} + 2h_{xz}\alpha + 2\eta_{xz}\alpha)t + O(t^2),
\end{aligned}
\tag{3.27}
$$

and

$$
\begin{aligned}
R^2(t) = t^3 + \Big[&(1/3)\alpha^2 + (1/3)\alpha\beta + (1/3)\beta^2 + (1/6)\eta_{xz}h_{xz} - (1/6)\eta_{yz}h_{yz} + (1/12)\eta_{xz}^2 + (1/12)\eta_{yz}^2 \\
&+ (1/12)h_{xz}^2 + (1/12)h_{yz}^2 + (1/3)h_{xy}^2\Big] t^5 + O(t^6).
\end{aligned}
\tag{3.28}
$$

These expansions are useful in numerically computing the solution for short times because they are cheaper than the full expressions in (3.24) and (3.25). Also they can be used to show that the solution obtained satisfies the expected singularity of our solution near $t = 0$

$$
S(t, x, y, z) \longrightarrow Q\,\delta(x)\,\delta(y)\,\delta(z)\ (t \longrightarrow 0). \tag{3.29}
$$

3.4 Apparent coefficient of the diffusion

We define the apparent coefficient of diffusion that combines the effects in the inhomogeneity of the mean flow with that of the turbulent diffusion coefficient A by

$$K_a \equiv \frac{1}{4}\frac{d\sigma^2}{dt}, \tag{3.30}$$

where

$$\sigma^2 \equiv (\sigma_1^2(t)\,\sigma_2^2(t)\,\sigma_3^2(t))^{1/3}, \tag{3.31}$$

with $\sigma_1(t)$, $\sigma_2(t)$ and $\sigma_3(t)$ being the variances in the principal axes.

Proposition 2. *$\sigma_1(t)\sigma_2(t)\sigma_3(t) = 8\,A^{3/2}\,R(t)$ where $R(t)$ is defined in (3.25) and (A.7).*

Proof. The Eulerian solution (3.23) has the form

$$S\,(t,x,y,z) = \frac{Q}{8(A\pi)^{3/2}R(t)} e^{\vec{x}^T M\vec{x}}$$

where

$$\mathbf{M} = \begin{bmatrix} \dfrac{C_{x^2}}{4AR^2(t)} & \frac{1}{2}\dfrac{C_{xy}}{4AR^2(t)} & \frac{1}{2}\dfrac{C_{xz}}{4AR^2(t)} \\ \frac{1}{2}\dfrac{C_{xy}}{4AR^2(t)} & \dfrac{C_{y^2}}{4AR^2(t)} & \frac{1}{2}\dfrac{C_{yz}}{4AR^2(t)} \\ \frac{1}{2}\dfrac{C_{xz}}{4AR^2(t)} & \frac{1}{2}\dfrac{C_{yz}}{4AR^2(t)} & \dfrac{C_{z^2}}{4AR^2(t)} \end{bmatrix} \tag{3.32}$$

is the symmetric matrix of coefficients. By diagonalizing the matrix **M**

$$\mathbf{M} = \mathbf{R}\mathbf{D}\mathbf{R}^T, \tag{3.33}$$

and defining the vector $\vec{X}$ such that $\vec{X} = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \mathbf{R}^T\,\vec{x}$, the solution is put in a diagonal form

$$S\,(t,x,y,z) = \frac{Q}{8(A\pi)^{3/2}R(t)} e^{-\left(\frac{X_1^2}{\sigma_1^2(t)}+\frac{X_2^2}{\sigma_2^2(t)}+\frac{X_3^2}{\sigma_3^2(t)}\right)}, \tag{3.34}$$

We use conservation of mass

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} S\,(t,X_1,X_2,X_3)\,dX_1\,dX_2\,dX_3 = Q, \tag{3.35}$$

so that

$$\frac{Q}{8(A\pi)^{3/2}R(t)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-\left(\frac{X_1^2}{\sigma_1^2(t)}+\frac{X_2^2}{\sigma_2^2(t)}+\frac{X_3^2}{\sigma_3^2(t)}\right)}dX_1\,dX_2\,dX_3=Q. \tag{3.36}$$

Now using the fact that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-\left(\frac{X_1^2}{\sigma_1^2(t)}+\frac{X_2^2}{\sigma_2^2(t)}+\frac{X_3^2}{\sigma_3^2(t)}\right)}dX_1\,dX_2\,dX_3=\pi^{3/2}\sigma_1(t)\sigma_2(t)\sigma_3(t), \tag{3.37}$$

the results follows. Now we have

$$K_a = A\,\frac{d}{dt}\{(R^2(t))^{1/3}\}. \tag{3.38}$$

□

In case of a non isotropic diffusivity, we get

$$\sigma_1(t)\sigma_2(t)\sigma_3(t) = 8\,B^{1/2}A^{1/2}R(t), \tag{3.39}$$

and the apparent coefficient of diffusion is reduced to

$$K_a = A^{2/3}\,B^{1/3}\,\frac{d}{dt}.\{(R^2(t))^{1/3}\} \tag{3.40}$$

3.5 Asymptotic behavior of the apparent coefficient of diffusion

To study the small asymptotic time behavior of K_a, we use Taylor series around $t = 0$ for the apparent diffusion of coefficient

$$K_a = A\Big[1+\frac{1}{3}\Big(\alpha^2+\alpha\beta+\beta^2+(1/4)(h_{yz}-\eta_{yz})^2+(1/4)(h_{xz}-\eta_{xz})^2\Big)t^2\Big]+O(t^4). \tag{3.41}$$

The leading order term shows that for small times, the diffusion by small scales eddies is dominant. As t increases, the advection effects accumulate and could eventually dominate the diffusion by small eddies, depending on the flow.

To explore the large asymptotic time behavior of K_a, we write $R^2(t)$ in terms of the eigenvalues defined in (3.7).

$$\begin{aligned}
R^2(\alpha,\beta,\vec{h},\vec{\eta})(t) = {} & R_1(\alpha,\beta,\vec{h},\vec{\eta}) \cosh\Big((\lambda_2+\frac{\lambda_1}{2})t\Big)\Big(e^{\frac{\lambda_1 t}{2}} - e^{\frac{-\lambda_1 t}{2}}\Big) \\
& + R_2(\alpha,\beta,\vec{h},\vec{\eta}) \cosh\Big((2\lambda_2+\lambda_1)t\Big)\Big(e^{\lambda_1 t} - e^{-\lambda_1 t}\Big) \\
& + \frac{R_3}{\sqrt{M}}(\alpha,\beta,\vec{h},\vec{\eta}) \Big\{ \sinh\Big((2\lambda_2+\lambda_1)t\Big)\Big(e^{\lambda_1 t} + e^{-\lambda_1 t}\Big) - 2\sinh\Big((\lambda_2+\frac{\lambda_1}{2})t\Big)\Big(e^{\frac{\lambda_1 t}{2}} + e^{\frac{-\lambda_1 t}{2}}\Big)\Big\} \\
& + R_4(\alpha,\beta,\vec{h},\vec{\eta})\Big(e^{\lambda_1 t} - e^{-\lambda_1 t}\Big) + R_5(\alpha,\beta,\vec{h},\vec{\eta})\Big(e^{2\lambda_1 t} - e^{-2\lambda_1 t}\Big)
\end{aligned}$$

Proposition 3. *Regime 1: In case of $\lambda_1 = \gamma = 0$, and $M < 0$, the apparent coefficient of diffusion remains bounded.*

Proof. Using the following relation

$$R_1(\alpha,\beta,\vec{h},\vec{\eta}) + 2R_2(\alpha,\beta,\vec{h},\vec{\eta}) + 2R_4(\alpha,\beta,\vec{h},\vec{\eta}) + 4R_5(\alpha,\beta,\vec{h},\vec{\eta}) = 0,$$

$R^2(t)$ when removing γ, simplifies to

$$\begin{aligned}
R^2(t) = {} & \tilde{R}_1(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cosh\frac{\sqrt{M}t}{2} - 1\Big)t + \tilde{R}_2(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cosh\sqrt{M}t - 1\Big)t \\
& + \frac{\tilde{R}_3}{\sqrt{M}}(\alpha,\beta,\vec{h},\vec{\eta})\Big(\sinh\sqrt{M}t - 2\sinh\frac{\sqrt{M}t}{2}\Big) + \tilde{R}_4(\alpha,\beta,\vec{h},\vec{\eta})t^3,
\end{aligned}$$

where

$$\begin{aligned}
\tilde{R}_1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{128(A''P'^2 + B''P^2 + 2MC''PP')}{M^5} + \frac{1024(PQ'-P'Q)^2}{M^6}, \\
\tilde{R}_2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{8(\alpha^2 + h_{xy}^2)}{M^2} + \frac{128(PQ'-P'Q)^2}{M^6} + \frac{32(A'P'^2 + B'P^2 + 2C'PP')}{M^4}, \\
\tilde{R}_3(\alpha,\beta,\vec{h},\vec{\eta}) &= -\frac{1024(PQ'-P'Q)^2}{M^6\sqrt{M}} - \frac{128(A'P'^2 + B'P^2 + 2C'PP')}{M^4\sqrt{M}}, \\
\tilde{R}_4(\alpha,\beta,\vec{h},\vec{\eta}) &= -\frac{64(PQ'-P'Q)^2}{M^5} - \frac{16(A''P'^2 + B''P^2 + 2C''PP')}{M^4} - \frac{4\eta_{xy}^2}{M}, \qquad (3.42)
\end{aligned}$$

and where A, A', B, B', B'', C, C', C'', P, P', Q, Q' are defined in Eq. (3.21) and (3.11). Since $M = 4(\alpha^2 + h_{xy}^2 - \eta_{xy}^2) < 0$, the hyperbolic functions turn into sines and cosines:

$$\begin{aligned}
R^2(t) = {} & \tilde{R}_1(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cos\frac{\sqrt{|M|}t}{2} - 1\Big)t + \tilde{R}_2(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cos\sqrt{|M|}t - 1\Big)t \\
& + \frac{\tilde{R}_3(\alpha,\beta,\vec{h},\vec{\eta})}{\sqrt{|M|}}\Big(\sin\sqrt{|M|}t - 2\sin\frac{\sqrt{|M|}t}{2}\Big) + t^3\tilde{R}_4(\alpha,\beta,\vec{h},\vec{\eta}),
\end{aligned}$$

(3.43)

from which we can easily infer that K_a remains bounded. In fact, we can easily obtain

$$K_a = A\Bigg[3t^2\,\tilde{R}_4(\alpha,\beta,\vec{h},\vec{\eta}) + \tilde{R}_1(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cos\frac{\sqrt{|M|}t}{2} - \frac{\sqrt{|M|}\sin\sqrt{|M|}t}{2}\,t - 1\Big)$$
$$\tilde{R}_2(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cos\sqrt{|M|}t - (\sqrt{|M|}\,\sin\sqrt{|M|}t)\,t - 1\Big) + \tilde{R}_3(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cos\sqrt{|M|}t - \cos\frac{\sqrt{|M|}t}{2}\Big)\Bigg] \Bigg/$$
$$3\Bigg[t^3\tilde{R}_4(\alpha,\beta,\vec{h},\vec{\eta}) + \tilde{R}_1(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cos\frac{\sqrt{|M|}t}{2} - 1\Big)t + \tilde{R}_2(\alpha,\beta,\vec{h},\vec{\eta})\Big(\cos\sqrt{|M|}t - 1\Big)t$$
$$+\frac{\tilde{R}_3(\alpha,\beta,\vec{h},\vec{\eta})}{\sqrt{|M|}}\Big(\sin\sqrt{|M|}t - 2\sin\frac{\sqrt{|M|}t}{2}\Big)\Bigg]^{2/3}$$
$$\to A\,\tilde{R}_4^{1/3}, (t\to\infty). \qquad (3.44)$$

□

Regime 2: $M > 0$, or $\lambda_1 = \gamma \neq 0$, the diffusivity grows exponentially for large times, as is clear from inspecting (3.25)

Chapter Four
Illustrations

In this chapter, we illustrate how our solution and apparent coefficient of diffusion reduce to simple forms, for special linear flows.

- **Rotation**: the parameter space is such that $\alpha = \beta = \gamma = \eta_{yz} = \eta_{xz} = 0$, $\vec{h} = \vec{0}$, $\eta_{xy} > 0$, $M < 0$.
  In this case the solution simplifies to

$$S\,(t, x, y, z) = \frac{Q}{8(A\pi)^{3/2} t^{3/2}} e^{-\frac{1}{4At}\{x^2+y^2+z^2\}} \ , \tag{4.1}$$

  implying that pure rotation does not change the coefficient of diffusion, i.e. $K_a = A$, $\forall t$. This result is consistent, when integrated over z with that presented in [2]

- **Pure stretching deformation**: the parameter space is such that $\gamma = \alpha > 0, \beta = -2\alpha, \vec{h} = \vec{\eta} = \vec{0},\ M > 0$. In this case, the coefficients in Eq. (3.23) simplify to

$$\begin{aligned}
&C_{x^2}(t) = C_{z^2}(t) = \frac{1}{8\alpha^2} e^{-2\alpha t}(1 - e^{-2\alpha t})(e^{4\alpha t} - 1),\\
&C_{y^2}(t) = \frac{1}{4\alpha^2} e^{4\alpha t}(1 - e^{-2\alpha t})^2,\\
&C_{xy}(t) = 0,\\
&C_{yz}(t) = 0,\\
&C_{xz}(t) = 0,
\end{aligned}$$

  and

$$R(t) = \left\{ \frac{1}{16\alpha^3} \left(1 - e^{-2\alpha t}\right)\left(1 - e^{4\alpha t}\right)\left(e^{-2\alpha t} - 1\right) \right\}^{1/2}. \tag{4.2}$$

  In this case, the apparent coefficient of diffusion grows exponentially

$$\frac{K_a}{A} \sim e^{\frac{4\alpha}{3} t}\ (t \longrightarrow \infty). \tag{4.3}$$

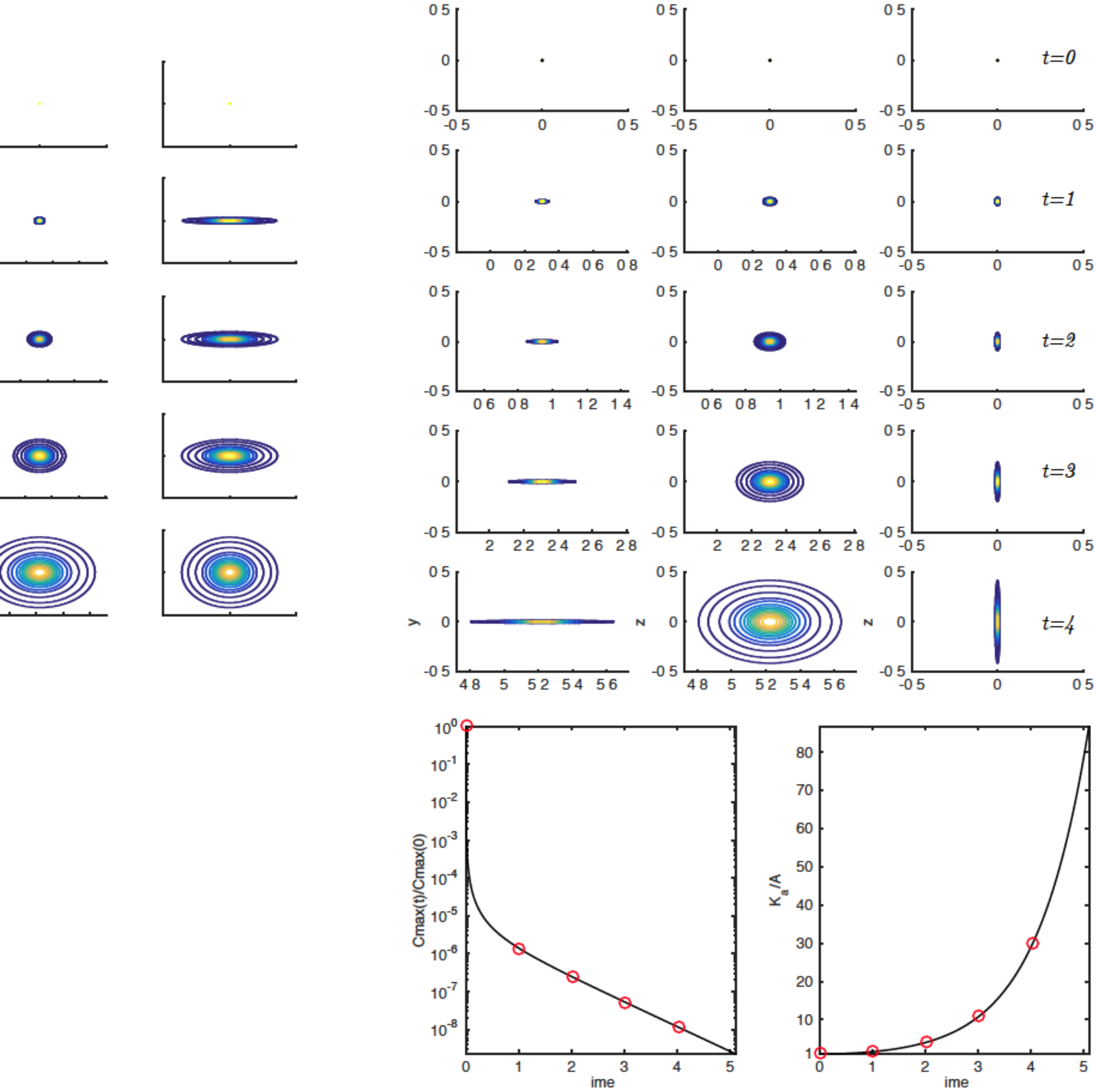


Figure 4.1 Stretching. Top: contours of concentration shown in the planes $z = 0, y = 0$ and $x = 0$ at different times. Lower left: decay of the normalized peak concentration with time. Lower right: normalized apparent coefficient of diffusion $\frac{K_a}{A}$ vs time.

As shown in Figure 4.1, the patch elongates equally in the x and z directions, which is consistent with $\alpha = \gamma > 0$ indicating that the patch expands in the $x - z$ plane. In contrast, diffusion in the y proceeds at a much lower rate, also consistent with $\beta < 0$. For these results, we took $U_0 = 0.2\,m/s$, $V_0 = W_0 = 0$, and $\alpha = 5 \times 10^{-5}\,/s$. The time and space axes are scaled according to $t_c = \frac{3}{4\alpha}$ and $L_c = U_0 \times t_c$. Note that in order to highlight the deformation phenomena, all the contour distributions presented in this section are scaled such that the concentration at the center of the patch is one in each time frame. The evolution of the actual peak concentration is presented in the lower left panel, where the red dots correspond to the times of the snapshots. In the lower right panel, we illustrate the exponential growth of the apparent coefficient of diffusion.

- **Uniform shear**: the parameter space is such that $\gamma = \alpha = \beta = h_{xz} = h_{yz} = \eta_{xz} = \eta_{xz} = 0$, $h_{xy} = -\eta_{xy} > 0$, $M = 0$. In this case, the coefficients in Eq. (3.23) simplify to

$$
\begin{aligned}
C_{x^2}(t) &= t^2, \\
C_{y^2}(t) &= t^2 + \frac{4}{3} h^2 t^4, \\
C_{z^2}(t) &= t^2 + \frac{h^2}{3} t^4 \\
C_{xy}(t) &= -2 h t^3 \\
C_{yz}(t) &= 0 \\
C_{xz}(t) &= 0
\end{aligned}
\tag{4.4}
$$

and

$$
R(t) = \left\{ \frac{h^2}{3} t^5 + t^3 \right\}^{1/2}. \tag{4.5}
$$

This gives an apparent diffusivity that grows like

$$
\frac{K_a}{A} \sim h^{2/3} t^{2/3}, \ (t \longrightarrow \infty). \tag{4.6}
$$

This result is consistent, when integrated over z with that presented in [2]

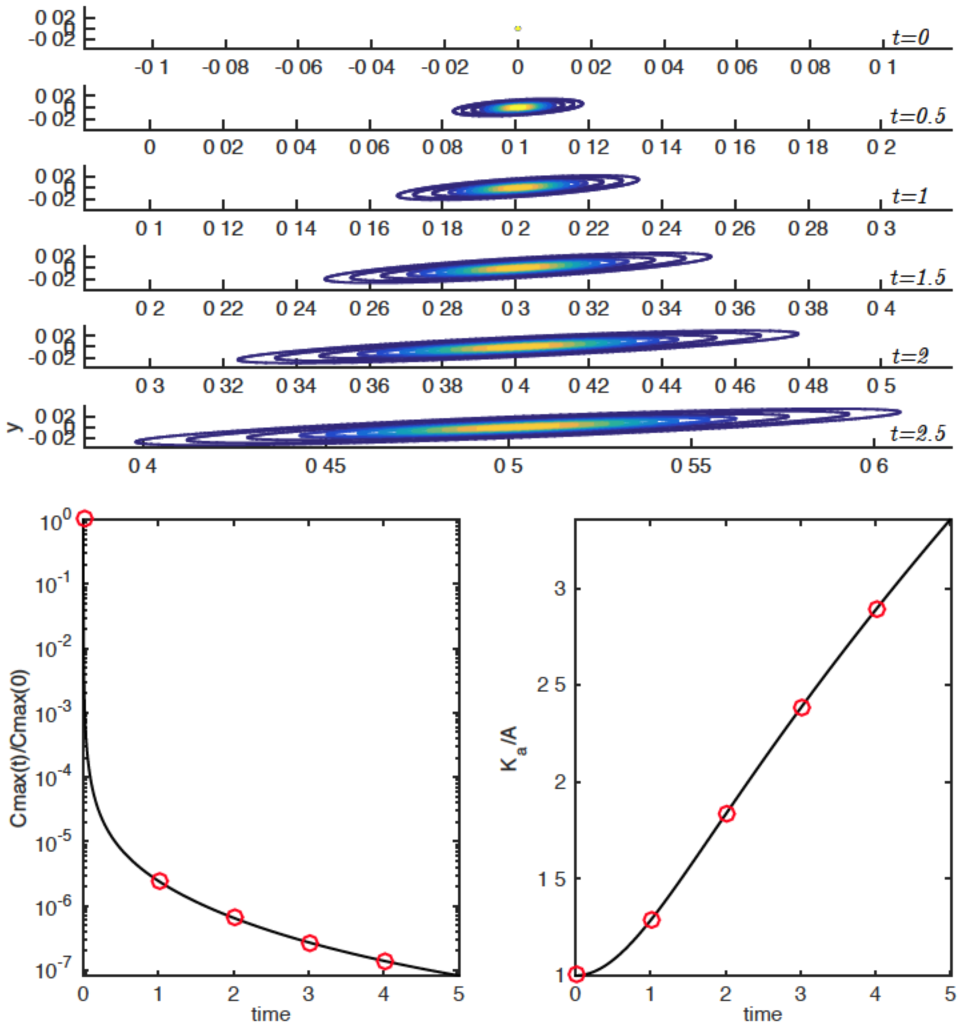


Figure 4.2 Shearing. Top: contours of concentration shown in the plane $z = 0$, at different times. Lower left: decay of the normalized peak concentration with time. Lower right: normalized apparent coefficient of diffusion $\frac{K_a}{A}$ vs time.

The top panel of Figure 4.2 shows snapshots of the concentration, where we observe the shearing of the patch in the $x-y$ plane at different times. For these results, we took $U_0 = 0.2\,m/s$, $V_0 = W_0 = 0$, and $h = 5\times10^{-5}/s$. The time and space axes are scaled according to $t_c = \frac{1}{h}$ and $L_c = U_0 \times t_c$. In the lower right panel, we show the growth of the apparent coefficient of diffusion as time goes by. Note that this $\sim t^{2/3}$ growth in K_a is slower than the exponential observed in the pure stretching case presented above.

- **Rotation and stretching**: the parameter space is such that $\gamma = \eta_{xz} = \eta_{yz} = 0$, $\vec{h} = 0$, $\alpha = -\beta > 0$, $\alpha < \eta_{xy}$. $M < 0$.

The coefficients become

$$
\begin{aligned}
C_{x^2}(t) = &-\frac{32}{M^2\sqrt{|M|}}\Big\{\Big(-\frac{\eta_{xy}^2\alpha^2 t}{4}\Big)\sin(2\sqrt{|M|}t) - \alpha t\Big(\frac{\alpha^3}{2} - \alpha\eta_{xy}^2 + \frac{\eta_{xy}^2 M t}{4}\Big)\sin(\sqrt{|M|}t)\\
&+\Big(\frac{\alpha\eta_{xy}^2\sqrt{|M|}t}{4}\Big)\cos^2(\sqrt{|M|}t) + \frac{\alpha\sqrt{|M|}t}{2}\Big(\frac{M}{8} + \alpha\eta_{xy}^2 t\Big)\cos(\sqrt{|M|}t) - \frac{\eta_{xy}^4\sqrt{M}}{2}t^2\\
&-\frac{\alpha^3\sqrt{|M|}}{4}t\Big\},
\end{aligned}
$$

$$
\begin{aligned}
C_{y^2}(t) = &-\frac{32}{M^2\sqrt{|M|}}\Big\{\Big(-\frac{\eta_{xy}^2\alpha^2 t}{4}\Big)\sin(2\sqrt{|M|}t) - \alpha t\Big(\frac{\alpha^3}{2} - \alpha\eta_{xy}^2 - \frac{\eta_{xy}^2 M t}{4}\Big)\sin(\sqrt{|M|}t)\\
&-\Big(\frac{\alpha\eta_{xy}^2\sqrt{|M|}t}{4}\Big)\cos^2(\sqrt{|M|}t) + \frac{\alpha\sqrt{|M|}t}{2}\Big(-\frac{M}{8} + \alpha\eta_{xy}^2 t\Big)\cos(\sqrt{|M|}t)\\
&-\frac{\eta_{xy}^4\sqrt{M}}{2}t^2 + \frac{\alpha^3\sqrt{|M|}}{4}t\Big\},
\end{aligned}
$$

$$
\begin{aligned}
C_{z^2}(t) &= -\frac{4\alpha\eta_{xy}}{M\sqrt{|M|}}\Big\{\sin(\sqrt{|M|}t) - \sqrt{|M|}\Big\},\\
C_{xy} &= -\frac{32\alpha\eta_{xy}^3 t}{M^2\sqrt{|M|}}\Big(\sin(\sqrt{|M|}t) - \sqrt{|M|}t\Big)\Big(\cos(\sqrt{|M|}t) - 1\Big),
\end{aligned}
\tag{4.7}
$$

and

$$
R(t) = \Big\{\frac{8\alpha^2 t}{M^2}\Big(\cos(\sqrt{|M|}t) - 1\Big) + \frac{4\eta_{xy}^2}{|M|}t^3\Big\}^{1/2}, \tag{4.8}
$$

which yields a bounded and oscillatory apparent coefficient of diffusion. Indeed, the bound in (3.44) simplifies to

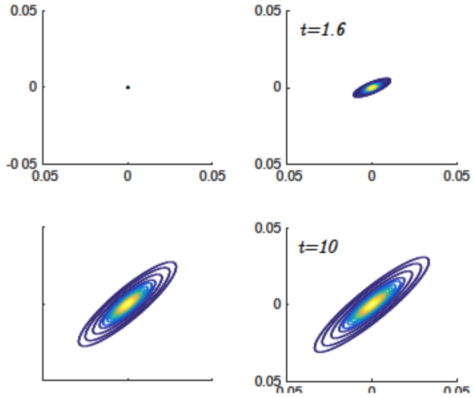
$$
\lim_{t\to\infty}\frac{K_a}{A} = \Big(\frac{\eta_{xy}^2}{|\alpha^2 - \eta_{xy}^2|}\Big)^{1/3}. \tag{4.9}
$$

Our three dimensional result in limit is consistent with the work of Okubo in two dimensions [2]. In fact, from his solution of $R(t)$, we can compute the apparent coefficient of diffusion for this case

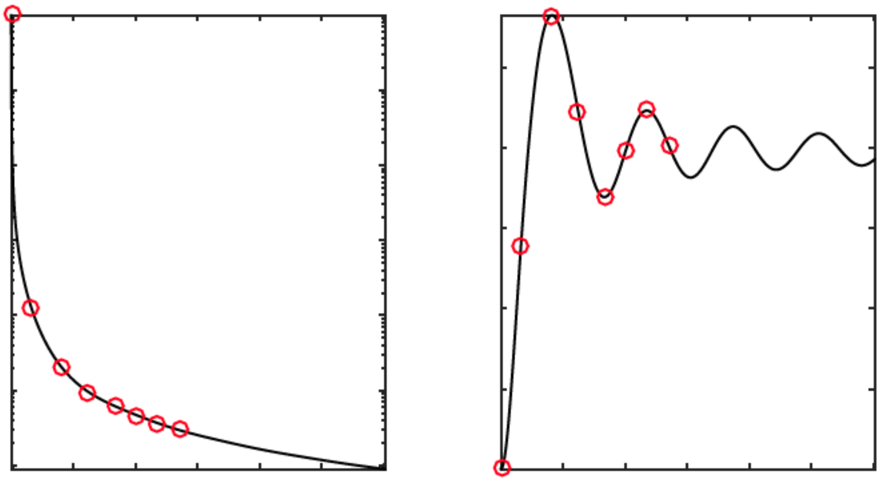
$$
K_a = \frac{1}{2}\frac{-\frac{(-1+\theta^2)\sin(2|M|t)}{|M|} + 2\theta^2 t}{\sqrt{-\frac{(-1+\theta^2)(\sin(|M|t))^2}{|M|^2} + \theta^2 t^2}}, \tag{4.10}
$$

where $\theta = \eta_{xy}/\sqrt{|\alpha^2 - \eta^2|}$, yielding an oscillatory behavior and the limit in two dimensions

$$
\frac{K_a}{A} \to \Big(\frac{\eta_{xy}^2}{|\alpha^2 - \eta_{xy}^2|}\Big)^{1/2}, (t\to\infty). \tag{4.11}
$$



0.05
0
-0 05
0.05
t=1.6
t=10



Chapter Five

A fundamental solution for an advection diffusion equation in a non uniform three dimensional flow

A fundamental solution for an advection diffusion equation in a non uniform three dimensional flow

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Abstract

In this paper, we develop an analytical solution for a three dimensional advection diffusion equation that models the evolution of the concentration of a passive tracer in a turbulent flow, where the mean flow is linear relative to the center of a patch of tracer, and where the effect of the small scale fluctuations can be modeled by an effective diffusivity coefficient using mixing length theory. The analytical solution relies on transforming the Eulerian equation into a system of equations for the characteristics and for the concentration expressed in the Lagrangian coordinates. From this solution, we infer an apparent coefficient of diffusion that combines the effect of differential advection by the mean flow and diffusion due to the small eddies. Using this fundamental solution within a numerical Lagrangian framework is expected to reduce the cost of solving the general advection diffusion equation in 3-D, specially when compared to methods that employ the solution in a uniform flow.

Keywords: mutli-dimensional advection diffusion, turbulent flow, eddy diffusivity, apparent coefficient of diffusion

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1. Introduction

The prediction of particle trajectories in the ocean is a task of great interest to multiple research communities, because of its important environmental applications, including pollutants spreading such as Lessepsian species, sewage outfalls, plastic garbage, and oil spills. This prediction also plays a role in explaining the spatial distribution of phytoplankton, which has effects on ecosystem stability and diversity [1] . The transport of passive tracers is governed by fluid dynamics equations capturing essential physical effects such as advection by geostrophic mesoscale eddies, and diffusion. Accurate numerical solution of these equations depends on several factors, the most challenging of which is the ability to resolve effects of turbulence because they are typically characterized by smaller scales than mean velocities; turbulence effects are captured in a parameter called eddy diffusivity [2].

The deterministic approach to quantify the effect of turbulence on tracer concentration consists of applying the famous Reynolds decomposition [3] to a time-homogeneous flow to obtain a (locally) time averaged advection diffusion equation that contains the effect of the fluctuations as $< u'C' >$, where primes denote fluctuating parts of concentration and velocity, and where brackets denote local time average. This leads to the classical closure problem, which consists of relating the fluctuating parts to the average concentration gradient through an "effective diffusivity", in a manner analogous to Fick's law of molecular diffusion. Many suggested semi-empirical closure approximations to deal with this problem, among which were ([4], [5] and [6]). The simplest approach is due to Prandtl. Even though Prandtl acknowledged the variety of scales in turbulence, he suggested a simplification by taking an average scale which is the mixing length.

We are interested here in mean flows, such as ocean flows, that can be locally resolved with a linear flow that captures essential physical effects such as rotation, deformation and shear [7]. In this paper, we present an analytic solution to an advection diffusion equation in three dimension, for the mean concentration of a tracer being advected by a turbulent ocean flow in which separation of scales is possible, and in which the mean flow is linear in space. Our work is an extension of the seminal work presented in two dimensions by Okubo in [8]. To our knowledge, this is the first analytical solution presented in three dimensions. This analytic solution is based on transforming the Eulerian equation into a system of ordinary differential equations that describe the trajectories (characteristics) and a diffusion equation for the concentration in the Lagrangian frame. The solution obtained shows that contours of concentration are ellipsoids with principal axes changing with time according to the linear flow parameters and to the diffusivity of the small eddies. From this solution, we obtain an apparent coefficient of diffusion that shows how the differential advection accentuates the diffusion due to the small eddies. We also analyze the limiting time behaviors of this apparent diffusion. We illustrate our solution with simple linear flows that capture the basic deformations (rotation, stretching, and shearing).

Solutions to the advection diffusion problem with a general mean velocity field can be obtained numerically. Eulerian and mesh dependent schemes such as finite difference methods (FDM), finite volume methods (FVM) and finite elements method (FEM) are all well established in the computation of multi-dimensional advection-diffusion problems. For a high Péclet number however, they suffer from nonphysical oscillations and excessive numerical diffusion [9]. Extreme mesh refinement may be one possible solution but it requires excessive computational requirements. Alternative formulations such as Lagrangian methods ([10], [11], [12]) are sought. Lagrangian methods advect particles along their trajectories according to the local velocity. We foresee that this solution can be employed in this context, where instead of the local uniform velocity, a linear one can be used.

This paper is structured as follows. In Section 2., we present the derivation of the fundamental solution in 3D. In Section 3., we infer from this solution the apparent coefficient of diffusion that shows the effects of the differential advection on the diffusivity. We also explore the small and large time asymptotics of this apparent diffusion. In Section 4. we present illustrations of the solution with simple linear flows.

2. Fundamental solution for the advection diffusion equation with a linear velocity in three dimensions

2.1. Governing equation for the concentration in a turbulent flow with linear mean

We are interested in the three dimensional advection diffusion equation in a turbulent flow where the spectrum of turbulence is separable into two parts: large scale and small scale eddies, with the scale of diffusion lying in between. The mean flow $\vec{U} = \left(U, V, W\right)$ due to the large eddies depends only on space. This simplifying assumption requires that the time scale over which the mean velocity varies is much larger than the observation time scale of the patch. The small scale eddies cause internal mixing. If the mixing is isotropic, their effect is to create an effective diffusion term with coefficient A that is the same in all directions, assumed to be a constant. In some flows, the diffusivity may not be isotropic. However, the case where the diffusion in the vertical direction is different from the horizontal can be dealt with a rescaling as presented in Appendix A.

The equation of interest is thus

$$\begin{aligned}
&\frac{\partial S}{\partial t} + U(x,y,z)\frac{\partial S}{\partial x} + V(x,y,z)\frac{\partial S}{\partial y} + W(x,y,z)\frac{\partial S}{\partial z} \\
&= A\left(\frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2} + \frac{\partial^2 S}{\partial z^2}\right) \qquad (1)
\end{aligned}$$

Since the flow can be locally resolved with a linear one, we may assume that this mean flow has components that are linear functions of the coordinates relative to the center of a small patch located an eddy that moves with velocity $\vec{U}_0$.

We may then write our governing equation for the concentration, in the moving reference frame, as follows

$$\begin{aligned}
&S_t + \left[\left(\frac{\partial U}{\partial x}\right)_0 x + \left(\frac{\partial U}{\partial y}\right)_0 y + \left(\frac{\partial U}{\partial z}\right)_0 z\right] S_x \\
&\left[\left(\frac{\partial V}{\partial x}\right)_0 x + \left(\frac{\partial V}{\partial y}\right)_0 y + \left(\frac{\partial V}{\partial z}\right)_0 z\right] S_y \\
&\left[\left(\frac{\partial W}{\partial x}\right)_0 x + \left(\frac{\partial W}{\partial y}\right)_0 y + \left(\frac{\partial W}{\partial z}\right)_0 z\right] S_z \\
&= A\,\Delta S, \qquad (2)
\end{aligned}$$

where the Laplacian is $\Delta S \equiv S_{xx} + S_{yy} + S_{zz}$.

The coefficients in the above Taylor expansion relate to meaningful physical quantities of the flow. We denote those by

$$\alpha = \left(\frac{\partial U}{\partial x}\right)_0, \quad \beta = \left(\frac{\partial V}{\partial y}\right)_0, \quad \gamma = \left(\frac{\partial W}{\partial z}\right)_0 : \text{stretching deformation} \tag{3}$$

$$\vec{h} = \begin{bmatrix} h_{xy} = \frac{1}{2}(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y})_0 \\ h_{xz} = \frac{1}{2}(\frac{\partial u}{\partial z})_0 \\ h_{yz} = \frac{1}{2}(\frac{\partial v}{\partial z})_0 \end{bmatrix} : \text{shearing deformation} \tag{4}$$

$$\vec{\eta} = \begin{bmatrix} \eta_{xy} = \frac{1}{2}(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y})_0 \\ \eta_{xz} = \frac{1}{2}(\frac{\partial u}{\partial z})_0 \\ \eta_{yz} = -\frac{1}{2}(\frac{\partial v}{\partial z})_0, \end{bmatrix} : \text{vorticity} \tag{5}$$

where the zero subscript indicates that they are evaluated at the center of the patch.

We assume non divergence in the mean velocity field, that is we have $\gamma = -\alpha - \beta$. Furthermore, we assume the vertical velocity component with respect to x and y are negligible that is $\frac{\partial W}{\partial x} = \frac{\partial W}{\partial y} = 0$.

The three dimensional Eulerian advection diffusion equation we want to solve is then

$$S_t + \Bigg(\alpha x + (h_{xy} - \eta_{xy})y + (h_{xz} + \eta_{xz})z\Bigg)S_x + \Bigg((h_{xy} + \eta_{xy})x + \beta y + (h_{yz} - \eta_{yz})z\Bigg)S_y + \big(\gamma z\big)S_z$$
$$= A\,\Delta S, \tag{6}$$

If we are looking for a fundamental solution, the initial condition is a delta function in space with strength Q

$$S(0, x, y, z) = Q\,\delta(x)\delta(y)\delta(z).$$

2 2. Derivation of the fundamental solution

2 2.1. Characteristics equations and Lagrangian equation for the concentration in the Lagrangian frame

We represent the solution $S(t, x, y, z)$ to Eq. (6) in a Lagrangian frame of reference

$$\Gamma(t, a, b, c) \equiv S(t, x(t, a, b, c), y(t, a, b, c), z(t, a, b, c)) \tag{7}$$

where a, b and c represent the initial coordinates of a particle, and where $x(t, a, b, c), y(t, a, b, c)$ and $z(t, a, b, c)$ are its coordinates at time t. With this representation, Eulerian Eq. (6) is equivalent to the following Lagrangian system for the displacements and the Lagrangian concentration:

$$\frac{d}{dt}\begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} = \mathbf{T}\begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} \tag{8}$$

$$\Gamma_t = A\Big([[\Gamma, y, z], y, z] + [x, [x, \Gamma, z], z] + [x, y, [x, y, \Gamma]]\Big) \tag{9}$$

where

$$\mathbf{T} = \begin{bmatrix} \alpha & h_{xy} - \eta_{xy} & h_{xz} + \eta_{xz} \\ h_{xy} + \eta_{xy} & \beta & h_{yz} - \eta_{yz} \\ 0 & 0 & \gamma \end{bmatrix},$$

where the bracket notation stands for the Jacobian, i.e. $[A, B, C] = \dfrac{\partial(A, B, C)}{\partial(a, b, c)}$. This is subject to the initial conditions $x = a$, $y = b$ and $z = c$ at $t = 0$, and $\Gamma(t = 0, a, b, c) = Q\,\delta(a)\delta(b)\delta(c)$.

In fact, from the basic relation relating Eulerian and Lagrangian quantities (7) and the chain rule, we easily see that

$$\Gamma_t = \frac{DS}{D\,t} = S_t + S_x\,x_t + S_y\,y_t + S_z\,z_t \tag{10}$$

Now using (8) and (6), we see that

$$\begin{aligned} \Gamma_t &= S_t + \mathbf{T}\begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} \cdot \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} \\ &= A\Delta S \end{aligned} \tag{11}$$

Expressing the partial derivatives of S in terms of those of Γ using the chain rule again, we see that

$$\begin{aligned} S_{xx} &= \big[[\Gamma, y, z], y, z\big] \\ S_{yy} &= [x, [x, \Gamma, z], z] \\ S_{zz} &= [x, y, [x, y, \Gamma]] \end{aligned} \tag{12}$$

2 2.2. Solution of the linear ODE system for the displacements

We diagonalize the system above (8). The eigenvalues are

$$
\begin{aligned}
\lambda_1 &= -\alpha - \beta = \gamma \\
\lambda_2 &= \frac{1}{2}\left[(\alpha+\beta) + \left((\alpha-\beta)^2 + 4(h_{xy}^2 - \eta_{xy}^2)\right)^{1/2}\right] \\
\lambda_3 &= \frac{1}{2}\left[(\alpha+\beta) - \left((\alpha-\beta)^2 + 4(h_{xy}^2 - \eta_{xy}^2)\right)^{1/2}\right].
\end{aligned} \tag{13}
$$

The corresponding eigenvectors are

$$
\begin{aligned}
\vec{V}_1 &= \begin{pmatrix} \frac{(\alpha+2\beta)(h_{xz}+\eta_{xz})-(h_{xy}-\eta_{xy})(h_{yz}-\eta_{yz})}{-2\alpha^2-2\beta^2-5\alpha\beta+h_{xy}^2-\eta_{xy}^2} \\ \frac{(2\alpha+\beta)(h_{yz}-\eta_{yz})-(h_{xy}+\eta_{xy})(h_{xz}+\eta_{xz})}{-2\alpha^2-2\beta^2-5\alpha\beta+h_{xy}^2-\eta_{xy}^2} \\ 1 \end{pmatrix} \\
\vec{V}_2 &= \begin{pmatrix} \frac{\alpha-\beta+\left((\alpha-\beta)^2+4(h_{xy}^2-\eta_{xy}^2)\right)^{1/2}}{2(h_{xy}+\eta_{xy})} \\ 1 \\ 0 \end{pmatrix} \\
\vec{V}_3 &= \begin{pmatrix} \frac{\alpha-\beta-\left((\alpha-\beta)^2+4(h_{xy}^2-\eta_{xy}^2)\right)^{1/2}}{2(h_{xy}+\eta_{xy})} \\ 1 \\ 0 \end{pmatrix}
\end{aligned} \tag{14}
$$

The coupled system is then solved explicitly

$$
\begin{aligned}
x(t;a,b,c) = {} & a e^{\frac{(\alpha+\beta)t}{2}}\left(\cosh\frac{\sqrt{M}t}{2} + \frac{\alpha-\beta}{\sqrt{M}}\sinh\frac{\sqrt{M}t}{2}\right) + \frac{2b}{\sqrt{M}}(h_{xy}-\eta_{xy})e^{\frac{(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2} \\
& + \frac{c}{S}\left[P\left(e^{\frac{(\alpha+\beta)t}{2}}\cosh\frac{\sqrt{M}}{2}t - e^{-(\alpha+\beta)t}\right) + e^{\frac{(\alpha+\beta)}{2}t}\frac{Q}{\sqrt{M}}\sinh\frac{\sqrt{M}}{2}t\right]
\end{aligned}
$$

$$
\begin{aligned}
y(t;a,b,c) = {} & b e^{\frac{(\alpha+\beta)t}{2}}\left(\cosh\frac{\sqrt{M}t}{2} - \frac{\alpha-\beta}{\sqrt{M}}\sinh\frac{\sqrt{M}t}{2}\right) + \frac{2a}{\sqrt{M}}(h_{xy}+\eta_{xy})e^{\frac{(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2} \\
& + \frac{c}{S}\left[P'\left(e^{\frac{(\alpha+\beta)t}{2}}\cosh\frac{\sqrt{M}}{2}t - e^{-(\alpha+\beta)t}\right) + e^{\frac{(\alpha+\beta)}{2}t}\frac{Q'}{\sqrt{M}}\sinh\frac{\sqrt{M}}{2}t\right]
\end{aligned}
$$

$$z(t;a,b,c) = ce^{-(\alpha+\beta)t}, \tag{15}$$

where

$$\begin{aligned} M &= (\alpha-\beta)^2 + 4(h_{xy}^2 - \eta_{xy}^2) \\ S &= -2(\alpha^2+\beta^2) - 5\alpha\beta + (h_{xy}^2 - \eta_{xy}^2) \\ P &= (h_{xy}-\eta_{xy})(h_{yz}-\eta_{yz}) - (h_{xz}+\eta_{xz})(\alpha+2\beta) \\ Q &= 2(h_{xy}-\eta_{xy})P' + (\alpha-\beta)P \\ P' &= (h_{xy}+\eta_{xy})(h_{xz}+\eta_{xz}) - (h_{yz}-\eta_{yz})(2\alpha+\beta) \\ Q' &= 2(h_{xy}+\eta_{xy})P - (\alpha-\beta)P'. \end{aligned} \tag{16}$$

Note that if $M = 0$, we replace, at this stage, $\frac{\sinh(\sqrt{M}t/2)}{\sqrt{M}}$ by $t/2$. Otherwise, we may assume $M \neq 0$.

2 2.3. Solution of the concentration in Lagrangian form

Equation (9) is a diffusion type equation in the a, b, c coordinates, so we shall solve it using Fourier transform. First we simplify its right hand side using the explicit dependence of the trajectories on a, b and c in (15).

$$\frac{\partial \Gamma}{\partial t} = A\Big(F_1(t)\Gamma_{aa} + F_2(t)\Gamma_{bb} + F_3(t)\Gamma_{cc} - 2G_1(t)\Gamma_{ab} - 2G_2(t)\Gamma_{ac} - 2G_3(t)\Gamma_{bc}\Big), \tag{17}$$

where the time dependent coefficients on the right hand side are given by

$$\begin{aligned} F_1(t) &= z_c^2(x_b^2+y_b^2) + (x_cy_b - x_by_c)^2 \\ F_2(t) &= z_c^2(x_a^2+y_a^2) + (x_ay_c - x_cy_a)^2 \\ F_3(t) &= (x_ay_b - x_by_a)^2 \\ G_1(t) &= z_c^2(x_ax_b + y_ay_b) - (x_ay_c - x_cy_a)(x_cy_b - x_by_c) \\ G_2(t) &= (x_ay_b - x_by_a)(x_cy_b - x_by_c) \\ G_3(t) &= (x_ay_b - x_by_a)(x_ay_c - x_cy_a) \end{aligned} \tag{18}$$

This equation is subject to $\Gamma(t=0,a,b,c) = Q\,\delta(a)\delta(b)\delta(c)$.

We apply the Fourier transform in the a, b, c variables

$$\hat{\Gamma}(t,w_1,w_2,w_3) = \frac{1}{8\pi^3}\int\int\int \Gamma(t,a,b,c)e^{-iw_1a-iw_2b-iw_3c}\,da\,db\,dc \tag{19}$$

to (17) to obtain the following equation governing the Fourier transform of Γ

$$\hat{\Gamma}_t = A\,\hat{\Gamma}\Big(-w_1^2F_1 - w_2^2F_2 - w_3^2F_3 + 2w_1w_2G_1 + 2w_1w_3G_2 + 2w_2w_3G_3\Big) \tag{20}$$

with solution

$$\hat{\Gamma}(t;w_1,w_2,w_3) = e^{-A\int\limits_0^t \Big(F_1w_1^2 + F_2w_2^2 + F_3w_3^2 - 2w_1w_2G_1 - 2w_1w_3G_2 - 2w_2w_3G_3\Big)\,d\tau} \times c(w_1,w_2,w_3) \tag{21}$$

where

$$c(w_1,w_2,w_3) = \frac{Q}{8\pi^3}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \delta(a)\delta(b)\delta(c)e^{iw_1a}e^{iw_2b}e^{iw_3c}\,da\,db\,dc \tag{22}$$

This yields the solution of the concentration in the Lagrangian frame of reference

$$\Gamma(t,a,b,c) = \frac{Q}{8(A\pi)^{3/2}R}\times \tag{23}$$
$$e^{-\frac{1}{4\,A\,R^2}\Big(a^2(\overline{F}_2\overline{F}_3-\overline{G}_3^2)+b^2(\overline{F}_1\overline{F}_3-\overline{G}_2^2)+c^2(\overline{F}_1\overline{F}_2-\overline{G}_1^2)+2ab(\overline{G}_2\overline{G}_3+\overline{G}_1\overline{F}_3)+2ac(\overline{G}_1\overline{G}_3+\overline{G}_2\overline{F}_2)+2bc(\overline{G}_1\overline{G}_2+\overline{G}_3\overline{F}_1\Big)}$$

where

$$\begin{aligned}
\overline{F}_1(t) &= \int_0^t F_1(\tau)d\tau \qquad (24)\\
\overline{F}_2(t) &= \int_0^t F_2(\tau)d\tau\\
\overline{F}_3(t) &= \int_0^t F_3(\tau)d\tau\\
\overline{G}_1(t) &= \int_0^t G_1(\tau)d\tau\\
\overline{G}_2(t) &= \int_0^t G_2(\tau)d\tau\\
\overline{G}_3(t) &= \int_0^t G_3(\tau)d\tau
\end{aligned}$$

and

$$R(t) = \left\{\overline{F}_1\overline{F}_2\overline{F}_3 - 2\overline{G}_1\overline{G}_2\overline{G}_3 - \overline{F}_2\overline{G}_2^2 - \overline{F}_3\overline{G}_1^2 - \overline{F}_1\overline{G}_3^2\right\}^{1/2} \qquad (25)$$

2 2.4. Solution in Eulerian form

After a tedious computation of the integrals term by term and their combination, we transform Eq. (23) back into Eulerian form $S(t, x, y, z)$. This manipulation involves inverting the ODE solutions Eq. (15) for a, b and c and collecting powers of x, y and z in Eq. (23). First we obtain a, b and c in terms of x, y and z

$$\begin{aligned}
a &= xe^{-\frac{(\alpha+\beta)t}{2}}\left(\cosh\frac{\sqrt{M}t}{2} - \frac{(\alpha-\beta)}{\sqrt{M}}\sinh\frac{\sqrt{M}t}{2}\right) - \frac{2y(h_{xy}-\eta_{xy})}{\sqrt{M}}e^{-\frac{(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2}\\
&+ z\left[\frac{P}{S}\left(e^{\frac{-(\alpha+\beta)t}{2}}\cosh\frac{\sqrt{M}t}{2} - e^{(\alpha+\beta)t}\right) - \frac{Q}{S\sqrt{M}}e^{\frac{-(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2}\right]\\
b &= ye^{-\frac{(\alpha+\beta)t}{2}}\left(\cosh\frac{\sqrt{M}t}{2} + \frac{(\alpha-\beta)}{\sqrt{M}}\sinh\frac{\sqrt{M}t}{2}\right) - \frac{2x(h_{xy}+\eta_{xy})}{\sqrt{M}}e^{-\frac{(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2}\\
&+ z\left[\frac{P'}{S}\left(e^{\frac{-(\alpha+\beta)t}{2}}\cosh\frac{\sqrt{M}t}{2} - e^{(\alpha+\beta)t}\right) - \frac{Q'}{S\sqrt{M}}e^{\frac{-(\alpha+\beta)t}{2}}\sinh\frac{\sqrt{M}t}{2}\right]\\
c &= ze^{(\alpha+\beta)t}
\end{aligned}$$

The final solution is a Gaussian that assumes he form

$$S(t,x,y,z) = \frac{Q}{8(A\pi)^{3/2}R(t)} e^{-\frac{C_{x^2}(t)x^2 + C_{y^2}(t)y^2 + C_{z^2}(t)z^2 + C_{xy}(t)xy + C_{xz}(t)xz + C_{yz}(t)yz}{4AR^2(t)}} \tag{26}$$

along with coefficients defined as

$$\begin{aligned}
C_{x^2}(t) &= C_x^1(\alpha,\beta,\vec{h},\vec{\eta}) + C_x^2(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t} + C_x^3(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} \\
&+ C_x^4(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} + C_x^5(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t}\cosh\sqrt{M}t \\
&+ C_x^6(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} + C_x^7(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t}\cosh\sqrt{M}t \\
&+ C_x^8(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{-\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} + C_x^9(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t} \\
&+ C_x^{10}(\alpha,\beta,\vec{h},\vec{\eta})e^{2\gamma t}
\end{aligned}$$

$$\begin{aligned}
C_{y^2}(t) &= C_y^1(\alpha,\beta,\vec{h},\vec{\eta}) + C_y^2(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t} + C_y^3(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} \\
&+ C_y^4(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} + C_x^5(\alpha,\beta,h,\eta)e^{\gamma t}\cosh\sqrt{M}t \\
&+ C_y^6(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} + C_y^7(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t}\cosh\sqrt{M}t \\
&+ C_y^8(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{-\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} + C_y^9(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t} \\
&+ C_y^{10}(\alpha,\beta,\vec{h},\vec{\eta})e^{2\gamma t}
\end{aligned}$$

$$
\begin{aligned}
C_{z^2}(t) = {} & C_z^1(\alpha,\beta,\vec{h},\vec{\eta}) + C_z^2(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t} \\
& + C_z^3(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + C_z^4(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C_z^5(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t}\cosh\sqrt{M}t + C_z^6(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} \\
& + C_z^8(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t}\cosh\sqrt{M}t + C_z^8(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{-\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} \\
& + C_z^9(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{-\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + C_z^{10}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{-\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C_z^{11}(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t} + C_z^{12}(\alpha,\beta,\vec{h},\vec{\eta})e^{-2\gamma t} + C_z^{13}(\alpha,\beta,\vec{h},\vec{\eta})e^{2\gamma t}
\end{aligned}
$$

$$
\begin{aligned}
C_{xy}(t) = {} & C_{xy}^1(\alpha,\beta,\vec{h},\vec{\eta}) + C_{xy}^2(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t} \\
& + C_{xy}^3(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + C_{xy}^4(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C_{xy}^5(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t}\cosh\sqrt{M}t + C_{xy}^6(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} \\
& + C_{xy}^7(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t}\cosh\sqrt{M}t + C_{xy}^8(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{-\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} \\
& + C_{xy}^9(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t} + C_{xy}^{10}(\alpha,\beta,\vec{h},\vec{\eta})e^{2\gamma t}
\end{aligned}
$$

$$
\begin{aligned}
C_{yz}(t) = {} & C^1_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) + C^2_{yz}(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t} \\
& + C^3_{yz}(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + C^4_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^5_{yz}(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t}\cosh\sqrt{M}t + C^6_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^7_{yz}(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t}\cosh\sqrt{M}t + C^8_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{-\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^9_{yz}(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{-\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + C^{10}_{yz}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{-\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^{11}_{yz}(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t} + C^{12}_{yz}(\alpha,\beta,\vec{h},\vec{\eta})e^{2\gamma t}
\end{aligned}
$$

$$
\begin{aligned}
C_{xz}(t) = {} & C^1_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) + C^2_{xz}(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t} \\
& + C^3_{xz}(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + C^4_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^5_{xz}(\alpha,\beta,\vec{h},\vec{\eta})e^{\gamma t}\cosh\sqrt{M}t + C^6_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^7_{xz}(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t}\cosh\sqrt{M}t + C^8_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{-\gamma t}\sinh\sqrt{M}t}{\sqrt{M}} \\
& + C^9_{xz}(\alpha,\beta,\vec{h},\vec{\eta})e^{\frac{-\gamma t}{2}}\cosh\frac{\sqrt{M}t}{2} + C^{10}_{xz}(\alpha,\beta,\vec{h},\vec{\eta})\frac{e^{\frac{-\gamma t}{2}}\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}} \\
& + C^{11}_{xz}(\alpha,\beta,\vec{h},\vec{\eta})e^{-\gamma t} + C^{12}_{xz}(\alpha,\beta,\vec{h},\vec{\eta})e^{2\gamma t} \qquad (27)
\end{aligned}
$$

and

$$
\begin{aligned}
R^2(t) = &\, R_1(\alpha,\beta,\vec{h},\vec{\eta}) \cosh \frac{\sqrt{M}t}{2}\left(e^{\frac{\gamma t}{2}} - e^{\frac{-\gamma t}{2}}\right) \\
&+ R_2(\alpha,\beta,\vec{h},\vec{\eta}) \cosh \sqrt{M}t\left(e^{\gamma t} - e^{-\gamma t}\right) \\
&+ R_3(\alpha,\beta,\vec{h},\vec{\eta})\left(\frac{\sinh\sqrt{M}t}{\sqrt{M}}\left[e^{\gamma t}+e^{-\gamma t}\right] - \frac{2\sinh\frac{\sqrt{M}t}{2}}{\sqrt{M}}\left[e^{\frac{\gamma t}{2}}+e^{\frac{-\gamma t}{2}}\right]\right) \\
&+ R_4(\alpha,\beta,\vec{h},\vec{\eta})\left(e^{\gamma t} - e^{-\gamma t}\right) \\
&+ R_5(\alpha,\beta,\vec{h},\vec{\eta})\left(e^{2\gamma t} - e^{-2\gamma t}\right).
\end{aligned} \tag{28}
$$

Here, C_x^i, C_y^i, C_z^i, C_{xy}^i, C_{xz}^i, C_{yz}^i and $R_i(i = 1,..,13)$ depend only on the parameters of the flow $(\alpha,\beta,\vec{h},\vec{\eta})$ and are presented in Eq. (B.1) , Eq. (B.2), Eq. (B.3), Eq. (B.5), Eq. (B.7), Eq. (B.6) and Eq. (B.8) in Appendix B.

The form of the solution suggests that the contours of concentration are a set of ellipsoids with principal axes that vary in time, according to the parameters of the linear flow $(\alpha,\beta,\vec{h},\vec{\eta})$. The impact of differential advection on the deformation the patch can be assessed in terms of the following characteristics: an apparent coefficient of diffusion, orientation of the principal directions, and the mixing lengths, σ_1, σ_2 and σ_3 along these directions. In Section 3., we derive an expression for the apparent coefficient of diffusion and explore its small and large time asymptotic behavior.

2 2.5. Small time behavior of the solution

We explore the small time asymptotics of the solution which we first conveniently write in the form

$$
S(t,x,y,z) = \frac{Q}{8(A\pi)^{3/2}R(t)} e^{-\left(\frac{x^2}{\sigma^2_{x^2}(t)}+\frac{y^2}{\sigma^2_{y^2}(t)}+\frac{z^2}{\sigma^2_{z^2}(t)}+\frac{xy}{\sigma_{xy}(t)}+\frac{xz}{\sigma_{xz}(t)}+\frac{yz}{\sigma_{yz}(t)}\right)} \tag{29}
$$

Each coefficient is then expanded in a Taylor series around $t = 0$ as follows

$$
\begin{aligned}
\sigma^2_{x^2}(t) &= \frac{4AR^2(t)}{C_{x^2}(t)} \\
&= 4\,A\,t + 4\,A\,\alpha\,t^2 + \\
&4\,A\left[(2/3)\,\alpha^2 + (1/12)\,h_{xz}^2 - (1/3)\,h_{xy}^2 + (1/6)\,\eta_{xz}\,h_{xz} + (1/12)\,\eta_{xz}^2 - (2/3)\,h_{xy}\,\eta_{xy}\right] t^3 + O(t^4)
\end{aligned}
$$

$$
\begin{aligned}
\sigma^2_{y^2}(t) &= \frac{4AR^2(t)}{C_{y^2}(t)} \\
&= 4\,A\,t + 4\,A\,\beta\,t^2 + \\
&4\,A\left[(2/3)\beta^2 + (1/12)h_{yz}^2 - (1/3)h_{xy}^2 - (1/6)\eta_{yz}h_{yz} + (1/12)\eta_{yz}^2 + (2/3)h_{xy}\eta_{xy}\right] t^3 + O(t^4)
\end{aligned}
$$

$$
\begin{aligned}
\sigma^2_{z^2}(t) &= \frac{4AR^2(t)}{C_{z^2}(t)} \\
&= 4\,A\,t + 4\,A\,\gamma\,t^2 + \\
&4\,A\Big[(2/3)\,\alpha^2 + (4/3)\,\alpha\,\beta + (2/3)\,\beta^2 - (1/2)\,\eta_{xz}\,h_{xz} - (1/4)\,h_{yz}^2 - (1/4)\,h_{xz}^2 - (1/4)\,\eta_{xz}^2 \\
&+ (1/2)\,\eta_{yz}\,h_{yz} - (1/4)\,\eta_{yz}^2\Big] t^3 + O(t^4)
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{xy}(t) &= \frac{4AR^2(t)}{C_{xy}(t)} \\
&= -\frac{2\,A}{h_{xy}} + \\
&\frac{A}{6\,h_{xy}^2}\left(h_{xz}\,h_{yz} - \eta_{yz}\,h_{xz} + \eta_{xz}\,h_{yz} - \eta_{xz}\,\eta_{yz} - 4\,h_{xy}\,\beta - 4\,\beta\,\eta_{xy} - 4\,\alpha\,h_{xy} + 4\,\alpha\,\eta_{xy}\right) t + O(t^2)
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{yz}(t) &= \frac{4AR^2(t)}{C_{yz}(t)} \\
&= \frac{4\,A}{(\eta_{yz} - h_{yz})} + \\
&\frac{4\,A}{3(\eta_{yz} - h_{yz})^2}\left(-2\,h_{xy}\,h_{xz} - 2\,\eta_{xz}\,h_{xy} + \eta_{xy}\,h_{xz} + \eta_{xy}\,\eta_{xz} - 2\,h_{yz}\,\beta + 2\,\eta_{yz}\,\beta\right) t + O(t^2)
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{xz}(t) &= \frac{4AR^2(t)}{C_{xz}(t)} \\
&= -\frac{4\,A}{(h_{xz}+\eta_{xz})} - \\
&\frac{4\,A}{3\,(h_{xz}+\eta_{xz})^2}\left(2\,h_{xy}\,h_{yz} - 2\,h_{xy}\,\eta_{yz} + \eta_{xy}\,h_{yz} - \eta_{xy}\,\eta_{yz} + 2\,h_{xz}\,\alpha + 2\,\eta_{xz}\,\alpha\right)t + O(t^2)
\end{aligned}
\tag{30}
$$

and

$$
\begin{aligned}
R^2(t) = t^3 + \Big[&(1/3)\,\alpha^2 + (1/3)\,\alpha\,\beta + (1/3)\,\beta^2 + (1/6)\,\eta_{xz}\,h_{xz} - (1/6)\,\eta_{yz}\,h_{yz} + (1/12)\,\eta_{xz}^2 \\
&+ (1/12)\,\eta_{yz}^2 + (1/12)\,h_{yz}^2 + (1/12)\,h_{xz}^2 + (1/3)\,h_{xy}^2\Big]\,t^5 + O(t^6)
\end{aligned}
\tag{31}
$$

These expansions are cheaper to compute than the full expressions in Eq. (27) and Eq. (28), when one is interested in using the solution for short times. Also they can be used to show that, indeed, the solution obtained satisfies the expected singularity $t = 0$, i.e.

$$
S(t,x,y,z) \longrightarrow Q\,\delta(x)\,\delta(y)\,\delta(z) \;\; (t \longrightarrow 0). \tag{32}
$$

3. Apparent coefficient of diffusion

3.1. Obtaining the apparent diffusion from the solution

From our solution, we can get an apparent coefficient of diffusion

$$
K_a \equiv \frac{1}{4}\frac{d\sigma^2}{dt}, \tag{33}
$$

where a "mean variance" σ^2 is defined such that

$$
\sigma^2 \equiv \left(\sigma_1^2(t)\,\sigma_2^2(t)\,\sigma_3^2(t)\right)^{1/3}, \tag{34}
$$

with $\sigma_1(t)\,\sigma_2(t)$ and $\sigma_3(t)$ being the variances in the principal axes. The apparent coefficient of diffusion K_a shows the rate at which differential advection (encapsulated by the set of parameters of the flow $(\alpha, \beta, \vec{h}, \vec{\eta})$) magnifies the turbulent diffusion coefficient A.

To relate σ^2 to our solution, we first show that

$$\sigma_1(t)\,\sigma_2(t)\,\sigma_3(t) = 8\,A^{3/2}\,R(t), \tag{35}$$

using diagonalization. In fact, our solution can be put in diagonal form

$$S(t,x,y,z) = \frac{Q}{8(A\pi)^{3/2}R(t)} e^{-\left(\frac{X_1^2}{\sigma_1^2(t)}+\frac{X_2^2}{\sigma_2^2(t)}+\frac{X_3^2}{\sigma_3^2(t)}\right)}, \tag{36}$$

if we define $\vec{X} = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \mathbf{R}^T\vec{x}$. Here, the matrix $\mathbf{R}$ is defined such that

$$\mathbf{M} = \mathbf{R}\mathbf{D}\mathbf{R}^T, \tag{37}$$

where

$$\mathbf{M} = \begin{bmatrix} \frac{C_{x^2}}{4AR^2(t)} & \frac{1}{2}\frac{C_{xy}}{4AR^2(t)} & \frac{1}{2}\frac{C_{xz}}{4AR^2(t)} \\ \frac{1}{2}\frac{C_{xy}}{4AR^2(t)} & \frac{C_{y^2}}{4AR^2(t)} & \frac{1}{2}\frac{C_{yz}}{4AR^2(t)} \\ \frac{1}{2}\frac{C_{xz}}{4AR^2(t)} & \frac{1}{2}\frac{C_{yz}}{4AR^2(t)} & \frac{C_{z^2}}{4AR^2(t)} \end{bmatrix} \tag{38}$$

is the symmetric matrix of coefficients.

Now to show Eq. (35), we use conservation of mass

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} S(t,X_1,X_2,X_3)\,dX_1\,dX_2\,dX_3 = Q \tag{39}$$

so that

$$\frac{Q}{8(A\pi)^{3/2}R(t)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\left(\frac{X_1^2}{\sigma_1^2(t)}+\frac{X_2^2}{\sigma_2^2(t)}+\frac{X_3^2}{\sigma_3^2(t)}\right)}\,dX_1\,dX_2\,dX_3 = Q. \tag{40}$$

Now using the fact that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\left(\frac{X_1^2}{\sigma_1^2(t)}+\frac{X_2^2}{\sigma_2^2(t)}+\frac{X_3^2}{\sigma_3^2(t)}\right)}\,dX_1\,dX_2\,dX_3 = \pi^{3/2}\sigma_1(t)\,\sigma_2(t)\,\sigma_3(t), \tag{41}$$

the result follows.

So we have

$$K_a = A\,\frac{d}{dt}\{(R^2(t))^{1/3}\}, \tag{42}$$

with $R^2(t)$ given by Eqs. (28), (B.8).

3 2. Asymptotic behavior of K_a

We first explore the small time behavior of K_a. For this purpose, we expand K_a in a Taylor series around $t = 0$

$$K_a = A\left[1 + \frac{1}{3}\left(\alpha^2 + \alpha\,\beta + \beta^2 + (1/4)\,(h_{yz} - \eta_{yz})^2 + (1/4)\,(h_{xz} - \eta_{xz})^2\right) t^2\right] + O(t^4) \tag{43}$$

As expected and in qualitative agreement with the result in two dimensions, for small times, the diffusion by the small eddies is dominant. As time goes by, the differential advection effects accumulate and could eventually dominate the diffusion by the small eddies, depending on the flow.

Exploring the large time behavior depends on the specific parameters' space, specifically on the eigenvalues in Eq. (13). Whenever $\lambda_1 = \gamma = 0$, and $M < 0$, the apparent coefficient of diffusion remains bounded. In this case, upon removing γ, Eq. (28) and Eq. (B.8) simplify to

$$\begin{aligned} R^2(t) &= \tilde{R}_1(\alpha,\beta,\vec{h},\vec{\eta})\left(\cosh\frac{\sqrt{M}t}{2} - 1\right)t + \tilde{R}_2(\alpha,\beta,\vec{h},\vec{\eta})\left(\cosh\sqrt{M}t - 1\right)t \\ &\quad + \frac{\tilde{R}_3}{\sqrt{M}}(\alpha,\beta,\vec{h},\vec{\eta})\left(\sinh\sqrt{M}t - 2\sinh\frac{\sqrt{M}t}{2}\right) + \tilde{R}_4(\alpha,\beta,\vec{h},\vec{\eta})\,t^3 \end{aligned}$$

where

$$\begin{aligned} \tilde{R}_1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{128\big(A''P'^2 + B''P^2 + 2MC''PP'\big)}{M^5} + \frac{1024(PQ' - P'Q)^2}{M^6} \\ \tilde{R}_2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{8(\alpha^2 + h_{xy}^2)}{M^2} + \frac{128(PQ' - P'Q)^2}{M^6} + \frac{32\big(A'P'^2 + B'P^2 + 2C'PP'\big)}{M^4} \\ \tilde{R}_3(\alpha,\beta,\vec{h},\vec{\eta}) &= -\frac{1024(PQ' - P'Q)^2}{M^6\sqrt{M}} - \frac{128\big(A'P'^2 + B'P^2 + 2C'PP'\big)}{M^4\sqrt{M}} \\ \tilde{R}_4(\alpha,\beta,\vec{h},\vec{\eta}) &= -\frac{64(PQ' - P'Q)^2}{M^5} - \frac{16\big(A''P'^2 + B''P^2 + 2C''PP'\big)}{M^4} - \frac{4\eta_{xy}^2}{M} \end{aligned} \tag{44}$$

where $A, A', A'', B, B', B'', C, C', C'', P, P', Q, Q'$, are defined in Eq. (B.9). For $M < 0$, the hyperbolic functions turn into sines and cosines

$$R^2(t) = \tilde{R}_1(\alpha, \beta, \vec{h}, \vec{\eta})\left(\cos\left(\frac{\sqrt{|M|}t}{2}\right) - 1\right)t + \tilde{R}_2(\alpha, \beta, \vec{h}, \vec{\eta})\left(\cos\left(\sqrt{|M|}t\right) - 1\right)t$$
$$+ \frac{\tilde{R}_3}{\sqrt{|M|}}(\alpha, \beta, \vec{h}, \vec{\eta})\left(\sin\left(\sqrt{|M|}t\right) - 2\sin\left(\frac{\sqrt{|M|}t}{2}\right)\right) + \tilde{R}_4(\alpha, \beta, \vec{h}, \vec{\eta})\, t^3. \tag{45}$$

From this expression, we can easily infer that K_a remains bounded. In fact, we can also obtain

$$K_a \to A\, \tilde{R}_4^{1/3},\ (t \to \infty). \tag{46}$$

Whenever $M > 0$, or $\lambda_1 = \gamma \neq 0$, the apparent coefficient of diffusion grows exponentially for large times, as is clear from inspecting (28).

4. Illustrations

In this section, we illustrate how our solution and apparent coefficient of diffusion reduce to simple forms, for special linear flows. These flows capture the basic kinds of deformation (rotation, stretching, and shearing).

- **Rotation**: the parameter space is such that $\alpha = \beta = \gamma = \eta_{yz} = \eta_{xz} = 0$, $\vec{h} = \vec{0}$, $\eta_{xy} > 0$. $M < 0$. In this case the solution simplifies to

$$S(t, x, y, z) = \frac{Q}{8(A\pi)^{3/2}t^{3/2}} e^{-\frac{1}{4At}\{x^2+y^2+z^2\}} \tag{47}$$

  implying that pure rotation does not change the coefficient of diffusion, i.e. $K_a = A$, $\forall t$. Note that an integration over the z coordinate yields the corresponding two dimensional result presented in [8].

- **Pure stretching deformation**: the parameter space is such that $\gamma = \alpha > 0$, $\beta = -2\,\alpha$, $\vec{h} = \vec{\eta} = \vec{0}$, $M > 0$. In this case, the coefficients in Eq. (26) simplify to

$$
\begin{aligned}
C_{x^2}(t) &= C_{z^2}(t) = \frac{1}{8\,\alpha^2}\,e^{-2\,\alpha t}\big(1-e^{-2\alpha t}\big)\left(e^{4\,\alpha t}-1\right)\\
C_{y^2}(t) &= \frac{1}{4\,\alpha^2}\,e^{4\,\alpha t}\big(1-e^{-2\alpha t}\big)^2\\
C_{xy}(t) &= 0\\
C_{yz}(t) &= 0\\
C_{xz}(t) &= 0
\end{aligned}
$$

and

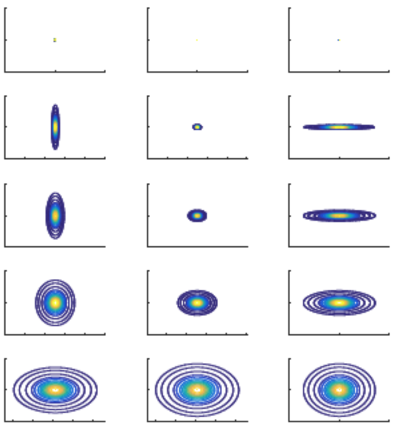
$$
R(t) = \left\{\frac{1}{16\,\alpha^3}\left(1-e^{-2\,\alpha\,t}\right)\left(1-e^{4\alpha\,t}\right)\left(e^{-2\alpha t}-1\right)\right\}^{1/2} \tag{48}
$$

In this case, the apparent coefficient of diffusion grows exponentially

$$
\frac{K_a}{A} \sim e^{\frac{4\,\alpha}{3}t}\ (t \longrightarrow \infty). \tag{49}
$$

As shown in Figure 1, the patch elongates equally in the x and z directions, which is consistent with $\alpha = \gamma > 0$ indicating that the patch expands in the $x-z$ plane. In contrast, diffusion in the y proceeds at a much lower rate, also consistent with $\beta < 0$. For these results, we took $U_0 = 0.2\,m/s$, $V_0 = W_0 = 0$, and $\alpha = 5\times10^{-5}\,/s.$. The time and space axes are scaled according to $t_c = \frac{3}{4\alpha}$ and $L_c = U_0 \times t_c$. Note that in order to highlight the deformation phenomena, all the contour distributions presented in this section are scaled such that the concentration at the center of the patch is one in each time frame. The evolution of the actual peak concentration is presented in the lower left panel, where the red dots correspond to the times of the snapshots. In the lower right panel, we illustrate the exponential growth of the apparent coefficient of diffusion.

- **Uniform shear**: the parameter space is such that $\gamma = \alpha = \beta = h_{xz} = h_{yz} = \eta_{xz} = \eta_{xz} = 0$, $h_{xy} = -\eta_{xy} > 0$. $M = 0$. In this case, the



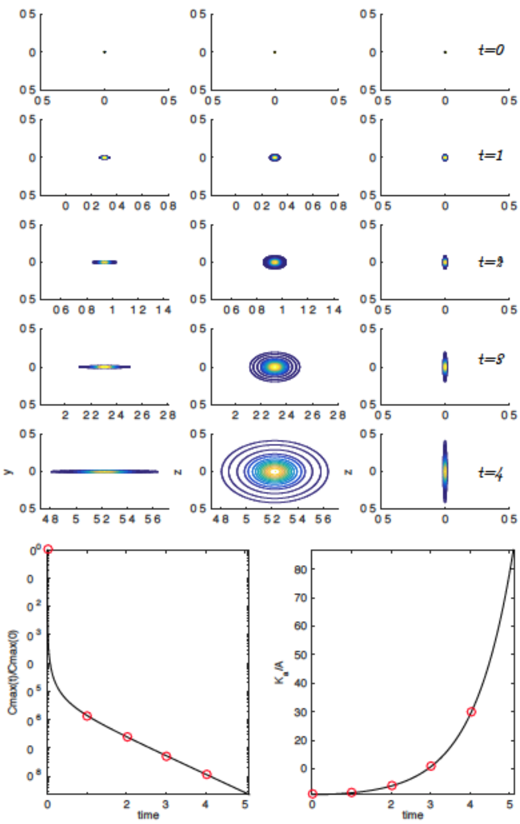


Figure 1: Stretching. Top: contours of concentration shown in the planes $z = 0, y = 0$ and $x = 0$ at different times. Lower left: decay of the normalized peak concentration with time. Lower right: normalized apparent coefficient of diffusion $\frac{K_a}{A}$ vs time.

coefficients in Eq. (26) simplify to

$$
\begin{aligned}
C_{x^2}(t) &= t^2 \\
C_{y^2}(t) &= t^2 + \frac{4}{3}\, h^2\, t^4 \\
C_{z^2}(t) &= t^2 + \frac{h^2}{3}\, t^4 \\
C_{xy}(t) &= -2\, h\, t^3 \\
C_{yz}(t) &= 0 \\
C_{xz}(t) &= 0
\end{aligned} \tag{50}
$$

and

$$
R(t) = \left\{ \frac{h^2}{3} t^5 + t^3 \right\}^{1/2} \tag{51}
$$

This gives an apparent diffusivity that grows like

$$
\frac{K_a}{A} \sim h^{2/3}\, t^{2/3}, \;\; (t \longrightarrow \infty). \tag{52}
$$

Note again here that an integration in z yields the corresponding two dimensional result presented in [8].

The top panel of Figure 2 shows snapshots of the concentration, where we observe the shearing of the patch in the $x - y$ plane at different times. For these results, we took $U_0 = 0.2\, m/s$, $V_0 = W_0 = 0$, and $h = 5 \times 10^{-5}\, /s$. The time and space axes are scaled according to $t_c = \frac{1}{h}$ and $L_c = U_0 \times t_c$. In the lower right panel, we show the growth of the apparent coefficient of diffusion as time goes by.

- **Rotation and stretching**: the parameter space is such that $\gamma = \eta_{xz} = \eta_{yz} = 0$, $\vec{h} = 0$, $\alpha = -\beta > 0$, $\alpha < \eta_{xy}$. $M < 0$.
  The coefficients become

$$
\begin{aligned}
C_{x^2}(t) = -\frac{32}{M^2 \sqrt{|M|}} \Bigg\{ & \left(-\frac{\eta_{xy}^2\, \alpha^2\, t}{4} \right) \sin\left(2\sqrt{|M|}t\right) - \alpha\, t \left(\frac{\alpha^3}{2} - \alpha\, \eta_{xy}^2 + \frac{\eta_{xy}^2\, M\, t}{4} \right) \sin\left(\sqrt{|M|}t\right) \\
& + \left(\frac{\alpha\, \eta_{xy}^2 \sqrt{|M|} t}{4} \right) \cos^2\left(\sqrt{|M|}t\right) + \frac{\alpha\, \sqrt{|M|}\, t}{2} \left(\frac{M}{8} + \alpha\, \eta_{xy}^2\, t \right) \cos\left(\sqrt{|M|}t\right) - \frac{\eta_{xy}^4\, \sqrt{M}}{2}\, t^2 \\
& - \frac{\alpha^3\, \sqrt{|M|}}{4}\, t \Bigg\}
\end{aligned}
$$

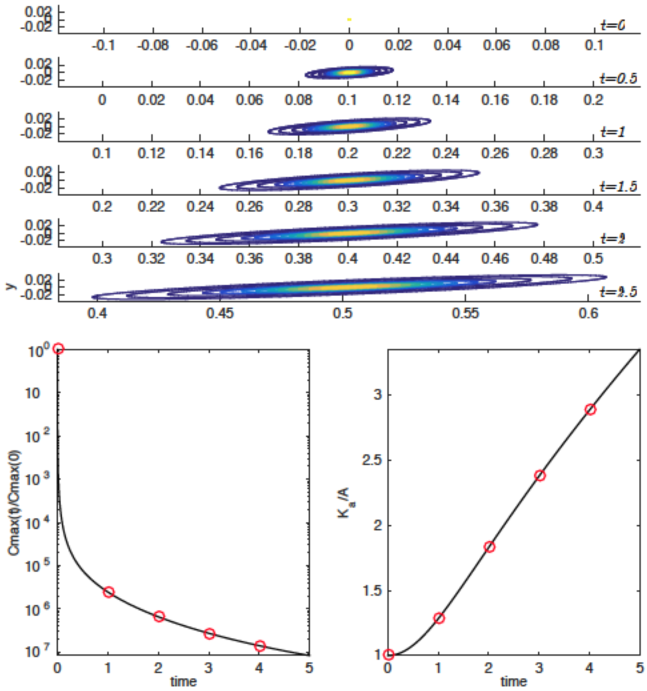


Figure 2: Shearing. Top: contours of concentration shown in the plane $z = 0$, at different times. Lower left: decay of the normalized peak concentration with time. Lower right: normalized apparent coefficient of diffusion $\frac{K_a}{A}$ vs time.

$$C_{y^2}(t) = -\frac{32}{M^2\sqrt{|M|}}\Big\{\Big(-\frac{\eta_{xy}^2\,\alpha^2\,t}{4}\Big)\sin(2\sqrt{|M|}t) - \alpha\,t\Big(\frac{\alpha^3}{2} - \alpha\,\eta_{xy}^2 - \frac{\eta_{xy}^2\,M\,t}{4}\Big)\sin(\sqrt{|M|}t)$$
$$-\Big(\frac{\alpha\,\eta_{xy}^2\sqrt{|M|}t}{4}\Big)\cos^2(\sqrt{|M|}t) + \frac{\alpha\sqrt{|M|}\,t}{2}\Big(-\frac{M}{8} + \alpha\,\eta_{xy}^2\,t\Big)\cos(\sqrt{|M|}t)$$
$$-\frac{\eta_{xy}^4\sqrt{M}}{2}\,t^2 + \frac{\alpha^3\sqrt{|M|}}{4}\,t\Big\}$$

$$
\begin{aligned}
C_{z^2}(t) &= -\frac{4\,\alpha\,\eta_{xy}}{M\sqrt{|M|}}\left\{\sin\left(\sqrt{|M|}t\right)-\sqrt{|M|}\right\}, && (53)\\
C_{xy}(t) &= -\frac{32\,\alpha\,\eta_{xy}^3\,t}{M^2\sqrt{|M|}}\left(\sin\left(\sqrt{|M|}t\right)-\sqrt{|M|}t\right)\left(\cos\left(\sqrt{|M|}t\right)-1\right),
\end{aligned}
$$

and

$$
R(t) = \left\{\frac{8\,\alpha^2\,t}{M^2}\left(\cos\left(\sqrt{|M|}t\right)-1\right)+\frac{4\eta_{xy}^2}{|M|}\,t^3\right\}^{1/2}. \tag{54}
$$

This case yields a bounded and oscillatory apparent coefficient of diffusion. Also, the limit in (46) simplifies to

$$
\frac{K_a}{A} \to \left(\frac{\eta_{xy}^2}{|\alpha^2-\eta_{xy}^2|}\right)^{1/3},\ (t\to\infty). \tag{55}
$$

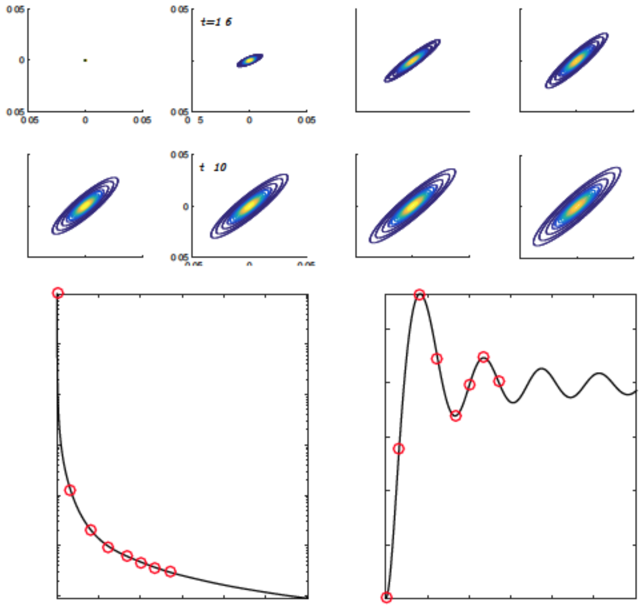
Qualitatively, this behavior is consistent by the findings of [8] in two dimensions. Although, this case is not displayed in Okubo's paper, we can compute, based on his solution (specifically based on his expression of $R(t)$) the apparent coefficient of diffusion in two dimensions

$$
K_a = \frac{1}{2}\,\frac{-\frac{\left(-1+\theta^2\right)\sin(2\,|M|\,t)}{|M|}+2\,\theta^2 t}{\sqrt{-\frac{(-1+\theta^2)(\sin(|M|\,t))^2}{|M|^2}+\theta^2t^2}} \tag{56}
$$

where $\theta = \eta_{xy}/\sqrt{|\alpha^2-\eta^2|}$, yielding an oscillatory behavior and the limit in two dimensions

$$
\frac{K_a}{A} \to \left(\frac{\eta_{xy}^2}{|\alpha^2-\eta_{xy}^2|}\right)^{1/2},\ (t\to\infty). \tag{57}
$$

We illustrate this behavior in the lower right panel of Figure 3 for the case $U_0 = V_0 = W_0 = 0, \alpha = -\beta = 5\times 10^{-5}\,/s$ and $\eta_{xy} = 1.1\,\alpha$. The time and space axes are scaled according to $t_c = \frac{1}{\alpha}$, $U_c = 1\,m/s$, and $L_c = U_c \times t_c$. The top panel of Figure 3 shows snapshots of the concentration in the $x-y$ plane at different times. In the figure, we observe that the patch undergoes limited stretching as it rotates to reach a 45 degrees angle, where it settles. This angle can be computed from the rotation matrix of Eq. (37) and the coefficients above.



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diffusion. We compute this coefficient and find that for small times, the small eddy diffusivity effect is dominant. The large time behavior depends on the parameters of the flow. If the motion is dominated by stretching for example, this coefficient grows. If the motion is dominated by rotation, the coefficient's growth is slower. We envision the future directions of this work to be focused on using our solution to simulate advection-diffusion of passive tracers in realistic flows. In these flows (i) the mean velocity is space and time dependent and (ii) the velocity profile, in the moving reference frame attached to the center of the patch, is nonlinear. To simulate the advection-diffusion of a patch in these flows, we tackle the first challenge by using a time stepping algorithm, where we deploy our solution over small time intervals, from t to $t + \Delta t$, during which the velocity of the patch's center is assumed to be constant. This entails restarting the problem every Δt. Note that since the solution is a Gaussian for any $t > 0$, the initial condition for the restarted problem is the Gaussian solution of the previous step. Also, and since convolving a Gaussian with a Gaussian yields another Gaussian with updated coefficients, then convolving boils down to updating the Gaussian's coefficients. The second challenge requires that the linear approximation in the moving reference frame to be not too much in error. This condition requires the sigmas of the patch to be smaller than the length scale characterizing departure from the linear profile (in the moving reference frame). This essentially puts a constraint on how large a patch can grow. One potential solution is to divide the patch into smaller ones as done in redistribution schemes.

6. Acknowledgments

This work was supported by LAU-CNRS grant 00844.

Appendix A. Non isotropic diffusivity

We consider an eddy diffusivity coefficient in the z-direction to be a constant $B \neq A$, where A is the horizontal eddy diffusivity, Eq. (2) becomes

$$
\begin{aligned}
&S_t + \left[\left(\frac{\partial U}{\partial x}\right)_0 x + \left(\frac{\partial U}{\partial y}\right)_0 y + \left(\frac{\partial U}{\partial z}\right)_0 z\right] S_x \\
&\left[\left(\frac{\partial V}{\partial x}\right)_0 x + \left(\frac{\partial V}{\partial y}\right)_0 y + \left(\frac{\partial V}{\partial z}\right)_0 z\right] S_y \\
&\left[\left(\frac{\partial W}{\partial x}\right)_0 x + \left(\frac{\partial W}{\partial y}\right)_0 y + \left(\frac{\partial W}{\partial z}\right)_0 z\right] S_z \\
&= A\,(S_{xx} + S_{yy}) + B\,S_{zz}
\end{aligned}
\tag{A.1}
$$

such that

$$S(0, x, y, z) = Q\,\delta(x)\delta(y)\delta(z).$$

Rescaling the above equation with $z^* = \sqrt{A/B}z$, and $w^* = \sqrt{A/B}w$ yields

$$
\begin{aligned}
&S_t + \left[\left(\frac{\partial U}{\partial x}\right)_0 x + \left(\frac{\partial U}{\partial y}\right)_0 y + \left(\frac{\partial U}{\partial z^*}\right)_0 z^*\right] S_x \\
&\left[\left(\frac{\partial V}{\partial x}\right)_0 x + \left(\frac{\partial V}{\partial y}\right)_0 y + \left(\frac{\partial V}{\partial z^*}\right)_0 z^*\right] S_y \\
&\left[\left(\frac{\partial W^*}{\partial x}\right)_0 x + \left(\frac{\partial W^*}{\partial y}\right)_0 y + \left(\frac{\partial W^*}{\partial z^*}\right)_0 z^*\right] S_{z^*} \\
&= A\,(S_{xx} + S_{yy} + S_{z^*z^*})
\end{aligned}
\tag{A.2}
$$

such that

$$S(0, x, y, z) = \sqrt{A/B}Q\,\delta(x)\delta(y)\delta(z).$$

So the solution methodology remains the same after rescaling. As for the apparent coefficient of diffusion in this case, it is straightforward to see that we get

$$\sigma_1(t)\,\sigma_2(t)\,\sigma_3(t) = 8\,B^{1/2}\,A^{1/2}\,R(t), \tag{A.3}$$

yielding

$$K_a = A^{2/3}\,B^{1/3}\,\frac{d}{dt}\{(R^2(t))^{1/3}\}, \tag{A.4}$$

Appendix B. Expressions for the constants in the coefficients

$$
\begin{aligned}
&C_x^1(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{B''}{2\gamma^2 M(M-\gamma^2)} \\
&+ \frac{(M-17\gamma^2)Q'^2 - (M^2 - 3M\gamma^2 + 18\gamma^4)P'^2 + 2\gamma(M+15\gamma^2)P'Q'}{4\gamma^2(M-\gamma^2)^2 S^2} \\
&C_x^2(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{Q'^2 - MP'^2}{\gamma^2 M(M-\gamma^2)S} + \frac{2\eta_{xy}(h_{xy}+\eta_{xy})}{\gamma^2 M} \\
&C_x^3(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{8(Q'-\gamma P')^2}{(M-\gamma^2)^2 S^2} \\
&C_x^4(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{-8(Q'-\gamma P')(\gamma Q' - MP')}{(M-\gamma^2)^2 S^2} \\
&C_x^5(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{-B}{2\gamma M(M-\gamma^2)} + \frac{-\gamma(7M+9\gamma^2)(Q'^2+MP'^2) + 2M(M+15\gamma^2)P'Q'}{4\gamma M(M-\gamma^2)^2 S^2} \\
&C_x^6(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{B'}{2\gamma(M-\gamma^2)} + \frac{(M+15\gamma^2)(Q'^2+MP'^2) - 2\gamma(7M+9\gamma^2)P'Q'}{4\gamma(M-\gamma^2)^2 S^2} \\
&C_x^7(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{-\gamma\big(Q'^2+MP'^2\big) - 2MP'Q'}{4\gamma M(M-\gamma^2)S^2} + \frac{B}{2\gamma M(M-\gamma^2)} \\
&C_x^8(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{-\big(Q'^2+MP'^2\big) - 2\gamma P'Q'}{4\gamma(M-\gamma^2)S^2} - \frac{B'}{2\gamma(M-\gamma^2)} \\
&C_x^9(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{-Q'^2+MP'^2}{4\gamma^2 MS^2} - \frac{2\eta_{xy}(h_{xy}+\eta_{xy})}{\gamma^2 M} \\
&C_x^{10}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{-B''}{2M\gamma^2(M-\gamma^2)} + \frac{-Q'^2 + (M-2\gamma^2)P'^2 - 2\gamma P'Q'}{4\gamma^2(M-\gamma^2)S^2}
\end{aligned}
\tag{B.1}
$$

$$
\begin{aligned}
C_y^1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{A''}{2\gamma^2 M(M-\gamma^2)} + \frac{(M-17\gamma^2)Q^2 - (M^2-3M\gamma^2+18\gamma^4)P^2 + 2\gamma(M+15\gamma^2)PQ}{4\gamma^2(M-\gamma^2)^2S^2}\\
C_y^2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{Q^2-MP^2}{\gamma^2M(M-\gamma^2)S} - \frac{2\eta_{xy}(h_{xy}-\eta_{xy})}{\gamma^2M}\\
C_y^3(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{8(Q-\gamma P)^2}{(M-\gamma^2)^2S^2}\\
C_y^4(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-8(Q-\gamma P)(\gamma Q-MP)}{(M-\gamma^2)^2S^2}\\
C_y^5(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-A}{2\gamma M(M-\gamma^2)} + \frac{-\gamma(7M+9\gamma^2)(Q^2+MP^2)+2M(M+15\gamma^2)PQ}{4\gamma M(M-\gamma^2)^2S^2}\\
C_y^6(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{A'}{2\gamma(M-\gamma^2)} + \frac{(M+15\gamma^2)(Q^2+MP^2)-2\gamma(7M+9\gamma^2)PQ}{4\gamma(M-\gamma^2)^2S^2}\\
C_y^7(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-\gamma\big(Q^2+MP^2\big)-2MPQ}{4\gamma M(M-\gamma^2)S^2} + \frac{A}{2\gamma M(M-\gamma^2)}\\
C_y^8(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-\big(Q^2+MP^2\big)-2\gamma PQ}{4\gamma(M-\gamma^2)S^2} - \frac{A'}{2\gamma(M-\gamma^2)}\\
C_y^9(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-Q^2+MP^2}{4\gamma^2MS^2} + \frac{2\eta_{xy}(h_{xy}-\eta_{xy})}{\gamma^2M}\\
C_y^{10}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-A''}{2M\gamma^2(M-\gamma^2)} + \frac{-Q^2+(M-2\gamma^2)P^2-2\gamma PQ}{4\gamma^2(M-\gamma^2)S^2}
\end{aligned}
\tag{B.2}
$$

$$
\begin{aligned}
C_z^1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{A''(Q'^2+9\gamma^2P'^2-6\gamma P'Q')+B''(Q^2+9\gamma^2P^2-6\gamma PQ)}{2\gamma^2M(M-\gamma^2)^2S^2} \qquad \text{(B.3)}\\
&+\frac{2MC''(QQ'+9\gamma^2PP'-3\gamma(PQ'+P'Q))}{2\gamma^2M(M-\gamma^2)^2S^2}+\frac{AB-C^2}{M^2(M-\gamma^2)^2}-\frac{4\eta_{xy}^2}{\gamma^2M}\\
C_z^2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)^2}{\gamma^2M(M-\gamma^2)S^3}+\frac{\eta_{xy}(PQ'-P'Q)}{\gamma^2MS^2}\\
C_z^3(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{4(PQ'-P'Q)^2}{(M-\gamma^2)^2S^4}-\frac{4P'^2(A''+MA')+4P^2(B''+MB')+8PP'(MC''+MC')}{M(M-\gamma^2)^2S^2}\\
C_z^4(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{2(M-3\gamma^2)(PQ'-P'Q)^2}{\gamma(M-\gamma^2)^2S^4}+\frac{4P'^2(\gamma^2A'+A'')+4P^2(\gamma^2B'+B'')+8PP'(\gamma^2C'+MC'')}{\gamma(M-\gamma^2)^2S^2}\\
C_z^5(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(7M+9\gamma^2)(PQ'-P'Q)^2}{4M(M-\gamma^2)^2S^4}-\frac{P^2B+P'^2A+2PP'C}{2\gamma M(M-\gamma^2)S^2}\\
C_z^6(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(M+15\gamma^2)(PQ'-P'Q)^2}{4\gamma(M-\gamma^2)^2S^4}+\frac{P^2B'+P'^2A'+2PP'C'}{2\gamma(M-\gamma^2)S^2}\\
C_z^7(\alpha,\beta,h,\eta) &= \frac{\big((M+11\gamma^2)A-4\gamma MA'\big)P'^2+\big((M+11\gamma^2)B-4\gamma MB'\big)P^2+2\big((M+11\gamma^2)C-4\gamma MC'\big)PP'}{2\gamma M(M-\gamma^2)^2S^2}\\
&-\frac{\gamma(7M+9\gamma^2)(PQ'-P'Q)^2}{4\gamma M(M-\gamma^2)^2S^4}+\frac{A''B+B''A-2MC''C}{\gamma M^2(M-\gamma^2)^2}\\
C_z^8(\alpha,\beta,h,\eta) &= \frac{-\big((M+7\gamma^2)A'-8\gamma A\big)P'^2-\big((M+7\gamma^2)B'-8\gamma B\big)P^2-2\big((M+7\gamma^2)C'-8\gamma C\big)PP'}{2\gamma(M-\gamma^2)^2S^2}\\
&-\frac{(M+15\gamma^2)(PQ'-P'Q)^2}{4\gamma(M-\gamma^2)^2S^4}\\
C_z^9(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{4(PQ'-P'Q)^2}{(M-\gamma^2)^2S^4}+\frac{4P'^2(A''+MA')+4P^2(B''+MB')+8PP'(MC''+MC')}{M(M-\gamma^2)^2S^2}\\
C_z^{10}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{4P'^2(\gamma^2A'-A''-2\gamma A)+4P^2(\gamma^2B'-B''-2\gamma B)+8PP'(\gamma^2C'-MC''-2\gamma C)}{\gamma(M-\gamma^2)^2S^2}\\
&-\frac{2(M-3\gamma^2)(PQ'-P'Q)^2}{\gamma(M-\gamma^2)^2S^4}\\
C_z^{11}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)^2}{\gamma^2M(M-\gamma^2)S^3}+\frac{4\eta_{xy}\big(PQ'-P'Q\big)}{\gamma^2M(M-\gamma^2)S}+\frac{8\eta_{xy}^2}{\gamma^2M}\\
&+\frac{(A''+\gamma A)P'^2+(B''+\gamma B)P^2+2(MC''+\gamma C)PP'}{\gamma^2M(M-\gamma^2)S^2}\\
C_z^{12}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(PQ'-P'Q)^2}{4\gamma^2(M-\gamma^2)S^4}+\frac{A''B''-M^2C''^2}{\gamma^2M^2(M-\gamma^2)^2}-\frac{\big((M-\gamma^2)A''+\gamma M(A+\gamma A')\big)P'^2}{\gamma^2M(M-\gamma^2)^2S^2}\\
&-\frac{\big((M-\gamma^2)B''+\gamma M(B+\gamma B')\big)P^2+2\big((M-\gamma^2)MC'+\gamma M(C+\gamma C')\big)PP'}{\gamma^2M(M-\gamma^2)^2S^2}\\
C_z^{13}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(PQ'-P'Q)^2}{4\gamma^2(M-\gamma^2)S^4}+\frac{-A''P'^2-B''P^2-2MC''PP'}{2\gamma^2M(M-\gamma^2)S^2} \qquad \text{(B.4)}
\end{aligned}
$$

$$
\begin{aligned}
C^1_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{MC''}{\gamma^2 M(M-\gamma^2)} + \frac{-(M-17\gamma^2)QQ' + (M^2-3M\gamma^2+18\gamma^4)PP' - \gamma(M+15\gamma^2)(PQ'+P'Q)}{2\gamma^2(M-\gamma^2)^2S^2} \\
C^2_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-2(QQ'-MPP')}{\gamma^2 M(M-\gamma^2)S} + \frac{-2\eta_{xy}(\alpha-\beta)}{\gamma^2 M} \\
C^3_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-16(Q-\gamma P)(Q'-\gamma P')}{(M-\gamma^2)S^2} \\
C^4_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{16\gamma QQ' + 16\gamma MPP' - 8(M+\gamma^2)(PQ'+P'Q)}{(M-\gamma^2)^2S^2} \\
C^5_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-C}{\gamma M(M-\gamma^2)} + \frac{\gamma(7M+9\gamma^2)(QQ'+MPP') - M(M+15\gamma^2)(PQ'+P'Q)}{2\gamma M(M-\gamma^2)^2S^2} \\
C^6_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{C'}{\gamma(M-\gamma^2)} + \frac{-(M+15\gamma^2)(QQ'+MPP') + \gamma(7M+9\gamma^2)(PQ'+P'Q)}{2\gamma(M-\gamma^2)S^2} \\
C^7_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\gamma\big(QQ'+MPP'\big) + M(PQ'+P'Q)}{2\gamma M(M-\gamma^2)S^2} + \frac{C}{\gamma M(M-\gamma^2)} \\
C^8_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(QQ'+MPP'\big) + \gamma(PQ'+P'Q)}{2\gamma(M-\gamma^2)S^2} - \frac{C'}{\gamma(M-\gamma^2)} \\
C^9_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(QQ'-MPP'\big)}{2\gamma^2 MS^2} + \frac{2\eta_{xy}(\alpha-\beta)}{\gamma^2 M} \\
C^{10}_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-MC''}{M\gamma^2(M-\gamma^2)} + \frac{QQ' - (M-2\gamma^2)PP' + \gamma(PQ'+P'Q)}{2\gamma^2(M-\gamma^2)^2S^2} \qquad \text{(B.5)}
\end{aligned}
$$

$$
\begin{aligned}
C^1_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-2(Q-3\gamma P)(PQ'-P'Q)}{\gamma^2(M-\gamma^2)^2S^2} + \frac{\big((M+3\gamma^2)P'-4\gamma Q'\big)A'' + \big((M+3\gamma^2)P-4\gamma Q\big)MC''}{M\gamma^2(M-\gamma^2)^2S}\\
C^2_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-2Q(PQ'-P'Q)}{M\gamma^2(M-\gamma^2)S^2} + \frac{-2\eta_{xy}Q}{\gamma^2MS}\\
C^3_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)\big(-12\gamma Q-2(M-11\gamma^2)P\big)}{\gamma(M-\gamma^2)^2S^3} + \frac{4(Q-\gamma P)MC''+4(Q'-\gamma P')A''}{\gamma M(M-\gamma^2)^2S}\\
C^4_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)\big(2(-M+7\gamma^2)Q-4\gamma(2M+3\gamma^2)P\big)}{\gamma(M-\gamma^2)^2S^3} - \frac{4(\gamma Q-MP)MC''+4(\gamma Q'-MP')A''}{\gamma M(M-\gamma^2)^2S}\\
C^5_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(-M(M+15\gamma^2)P+\gamma(7M+9\gamma^2)Q\big)\big(PQ'-P'Q\big)}{2\gamma M(M-\gamma^2)^2S^3} + \frac{PC+P'A}{\gamma M(M-\gamma^2)S}\\
C^6_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(-(M+15\gamma^2)Q+\gamma(7M+9\gamma^2)P\big)\big(PQ'-P'Q\big)}{2\gamma(M-\gamma^2)^2S^3} + \frac{PC'+P'A'}{\gamma(M-\gamma^2)S}\\
C^7_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(\gamma(5M+3\gamma^2)Q+(M+7\gamma^2)MP\big)(PQ'-P'Q)}{2\gamma M(M-\gamma^2)^2S^3}\\
&\quad + \frac{\big((M+3\gamma^2)A-4\gamma MA'\big)P' + \big((M+3\gamma^2)C-4\gamma MC'\big)P}{\gamma M(M-\gamma^2)^2S}\\
C^8_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big((M+7\gamma^2)Q+\gamma(5M+3\gamma^2)P\big)(PQ'-P'Q)}{2\gamma(M-\gamma^2)^2S^3}\\
&\quad + \frac{\big(-(M+3\gamma^2)A'+4\gamma A\big)P' + \big(-(M+3\gamma^2)C'+4\gamma C\big)P}{\gamma(M-\gamma^2)^2S}\\
C^9_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)\big(-4\gamma Q+2(M-3\gamma^2)P\big)}{\gamma(M-\gamma^2)^2S^3} + \frac{4(\gamma P-Q)MC''+4(\gamma P'-Q')A''}{\gamma M(M-\gamma^2)^2S}\\
C^{10}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(P'Q-PQ')\big(2(M-3\gamma^2)Q-4\gamma MP\big)}{2M\gamma^2(M-\gamma^2)S^3} + \frac{4\gamma(\gamma P'-Q')A'+4(\gamma P-Q)(\gamma C'-2\eta_{xy}(M-\gamma^2))}{\gamma(M-\gamma^2)^2S}\\
C^{11}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(P'Q-PQ')\big(-4\gamma MP+(M+3\gamma^2)Q\big)}{2M\gamma^2(M-\gamma^2)S^3} + \frac{2\eta_{xy}\big((M+3\gamma^2)Q-4\gamma MP\big)}{M\gamma^2(M-\gamma^2)S}\\
C^{12}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)(Q+\gamma P)}{2\gamma^2(M-\gamma^2)S^3} + \frac{-P'A''-PMC''}{\gamma^2M(M-\gamma^2)S} \qquad \text{(B.6)}
\end{aligned}
$$

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$$
\begin{aligned}
C^1_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{2(Q'-3\gamma P')(PQ'-P'Q)}{\gamma^2(M-\gamma^2)^2S^2} + \frac{\big((M+3\gamma^2)P'-4\gamma Q'\big)MC'' + \big((M+3\gamma^2)P-4\gamma Q\big)B''}{M\gamma^2(M-\gamma^2)^2S} \\
C^2_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{2Q'(PQ'-P'Q)}{M\gamma^2(M-\gamma^2)S^2} + \frac{2\eta_{xy}Q'}{\gamma^2MS} \\
C^3_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)\big(12\gamma Q'+2(M-11\gamma^2)P'\big)}{\gamma(M-\gamma^2)^2S^3} + \frac{4(Q-\gamma P)B''+4(Q'-\gamma P')MC''}{\gamma M(M-\gamma^2)^2S} \\
C^4_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)\big(2(M-7\gamma^2)Q'+4\gamma(2M+3\gamma^2)P'\big)}{\gamma(M-\gamma^2)^2S^3} - \frac{4(\gamma Q-MP)B''+4(\gamma Q'-MP')MC''}{\gamma M(M-\gamma^2)^2S} \\
C^5_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(M(M+15\gamma^2)P'-\gamma(7M+9\gamma^2)Q'\big)\big(PQ'-P'Q\big)}{2\gamma M(M-\gamma^2)^2S^3} - \frac{PB+P'C}{\gamma M(M-\gamma^2)S} \\
C^6_{xz}(\alpha,\beta,\vec{h},\vec{\eta} &= \frac{\big((M+15\gamma^2)Q'-\gamma(7M+9\gamma^2)P'\big)\big(PQ'-P'Q\big)}{2\gamma(M-\gamma^2)^2S^3} + \frac{PB'+P'C'}{\gamma(M-\gamma^2)S} \\
C^7_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-\big(\gamma(5M+3\gamma^2)Q'+(M+7\gamma^2)MP'\big)(PQ'-P'Q)}{2\gamma M(M-\gamma^2)^2S^3} \\
&\quad + \frac{\big((M+3\gamma^2)B-4\gamma MB'\big)P + \big((M+3\gamma^2)C-4\gamma MC'\big)P'}{\gamma M(M-\gamma^2)^2S} \\
C^8_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(-(M+7\gamma^2)Q'-\gamma(5M+3\gamma^2)P'\big)(PQ'-P'Q)}{2\gamma(M-\gamma^2)^2S^3} \\
&\quad + \frac{\big(-(M+3\gamma^2)B'+4\gamma B\big)P + \big(-(M+3\gamma^2)C'+4\gamma C\big)P'}{\gamma(M-\gamma^2)^2S} \\
C^9_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)\big(4\gamma Q'-2(M-3\gamma^2)P'\big)}{\gamma(M-\gamma^2)^2S^3} + \frac{4(\gamma P-Q)B''+4(\gamma P'-Q')MC''}{\gamma M(M-\gamma^2)^2S} \\
C^{10}_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)\big(-2(M-3\gamma^2)Q'+4\gamma MP'\big)}{\gamma(M-\gamma^2)^2S^3} \\
&\quad + \frac{4\gamma(\gamma P-Q)B'+4(\gamma P'-Q')(\gamma C'+2\eta_{xy}(M-\gamma^2)(\gamma P'-Q')}{\gamma(M-\gamma^2)^2S} \\
C^{11}_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(P'Q-PQ')\big(4\gamma MP'-(M+3\gamma^2)Q'\big)}{2M\gamma^2(M-\gamma^2)S^3} + \frac{2\eta_{xy}\big(-(M+3\gamma^2)Q'+4\gamma MP'\big)}{M\gamma^2(M-\gamma^2)S} \\
C^{12}_{xz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(PQ'-P'Q)(Q'+\gamma P')}{2\gamma^2(M-\gamma^2)S^3} + \frac{-PB''-P'MC''}{\gamma^2M(M-\gamma^2)S} \qquad \text{(B.7)}
\end{aligned}
$$

$$
\begin{aligned}
R_1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{8\big((M-\gamma^2)A''+2\gamma MA-2M\gamma^2A'\big)P'^2+8\big((M-\gamma^2)B''+2\gamma MB-2M\gamma^2B'\big)P^2}{\gamma M(M-\gamma^2)^3S^2} \\
&\quad+\frac{16\big((M-\gamma^2)MC''+2\gamma MC-2M\gamma^2C'\big)PP'}{\gamma M(M-\gamma^2)^3S^2}+\frac{4(M-5\gamma^2)(PQ'-P'Q)^2}{\gamma(M-\gamma^2)^3S^4} \\
R_2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(-\gamma(3M+5\gamma^2)A+M(M+7\gamma^2)A'\big)P'^2+\big(-\gamma(3M+5\gamma^2)B+M(M+7\gamma^2)B'\big)P^2}{\gamma M(M-\gamma^2)^3S^2} \\
&\quad+\frac{2\big(-\gamma(3M+5\gamma^2)C+M(M+7\gamma^2)C'\big)PP'}{\gamma M(M-\gamma^2)^3S^2}+\frac{\big(M^2+22M\gamma^2+9\gamma^4)\big)\big(PQ'-P'Q\big)^2}{4\gamma M(M-\gamma^2)^3S^4} \\
&\quad-\frac{AB-C^2}{\gamma M^2(M-\gamma^2)^2} \\
R_3(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\big(8\gamma A-4(M+\gamma^2)A'\big)P'^2+\big(8\gamma B-4(M+\gamma^2)B'\big)P^2+2\big(8\gamma C-4(M+\gamma^2)C'\big)PP'}{(M-\gamma^2)^3S^2} \\
&\quad-\frac{\big(2(M+3\gamma^2)\big(PQ'-P'Q\big)^2}{(M-\gamma^2)^3S^4} \\
R_4(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)^2}{\gamma^3M(M-\gamma^2)S^3}+\frac{4\eta_{xy}(PQ'-P'Q)}{\gamma^3M(M-\gamma^2)S}+\frac{4\eta_{xy}^2}{\gamma^3M}+\frac{\eta_{xy}(PQ'-P'Q)}{\gamma^3MS^2} \\
R_5(\alpha,\beta,\vec{h},\vec{\eta}) &= -\frac{\big((M-\gamma^2)A''+\gamma M(A+\gamma A')\big)P'^2+\big((M-\gamma^2)B''+\gamma M(B+\gamma B')\big)P^2}{2\gamma^3M(M-\gamma^2)^2S^2} \\
&\quad-\frac{2\big((M-\gamma^2)MC'+\gamma M(C+\gamma C')\big)PP'}{2\gamma^3M(M-\gamma^2)^2S^2}-\frac{M^2C''^2-A''B''}{2\gamma^3M^2(M-\gamma^2)^2}-\frac{(PQ'-P'Q)^2}{8\gamma^3(M-\gamma^2)S^4}
\end{aligned} \tag{B.8}
$$

where

$$
\begin{aligned}
M &= (\alpha-\beta)^2 + 4(h_{xy}^2 - \eta_{xy}^2) \\
S &= -2(\alpha^2+\beta^2) - 5\alpha\beta + (h_{xy}^2 - \eta_{xy}^2) \\
P &= (h_{xy}-\eta_{xy})(h_{yz}-\eta_{yz}) - (h_{xz}+\eta_{xz})(\alpha+2\beta) \\
Q &= 2(h_{xy}-\eta_{xy})P' + (\alpha-\beta)P \\
P' &= (h_{xy}+\eta_{xy})(h_{xz}+\eta_{xz}) - (h_{yz}-\eta_{yz})(2\alpha+\beta) \\
Q' &= 2(h_{xy}+\eta_{xy})P - (\alpha-\beta)P' \\
C &= 2h_{xy}(\alpha-\beta)^2 + 8h_{xy}(h_{xy}^2-\eta_{xy}^2) - 2\eta_{xy}(\alpha^2-\beta^2) \\
C' &= 2h_{xy}(\alpha+\beta) - 2\eta_{xy}(\alpha-\beta) \\
C'' &= 2h_{xy}(\alpha+\beta) - 2\eta_{xy}(\alpha-\beta) \\
A &= 2\beta(\alpha-\beta)^2 + 4h_{xy}(h_{xy}-\eta_{xy})(\alpha+\beta) - 4(h_{xy}^2-\eta_{xy}^2)(\alpha-\beta) \\
A' &= -2\beta(\alpha-\beta) + 4h_{xy}(h_{xy}-\eta_{xy}) \\
A'' &= -\gamma A - 4\eta_{xy}(h_{xy}-\eta_{xy})(M-\gamma^2) \\
B &= 2\alpha(\alpha-\beta)^2 + 4h_{xy}(h_{xy}+\eta_{xy})(\alpha+\beta) + 4(h_{xy}^2-\eta_{xy}^2)(\alpha-\beta) \\
B' &= 2\alpha(\alpha-\beta) + 4h_{xy}(h_{xy}+\eta_{xy}) \\
B'' &= -\gamma B + 4\eta_{xy}(h_{xy}+\eta_{xy})(M-\gamma^2) \qquad \text{(B.9)}
\end{aligned}
$$

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Chapter Six
Conclusion and Perspectives

We present in this thesis an analytical solution of the three dimensional advection diffusion equation in a turbulent flow where the mean velocity field is assumed to be non divergent and linear in space. We present in chapter 2 the mathematical background of the advection diffusion equation in a turbulent flow under the assumption of separation of scales using Reynolds decomposition. The equation that governs the mean concentration of a tracer advected with a non-divergent mean flow takes into account the inhomogeneity in the velocity field provided by the large scale eddies and the turbulence in the velocity due to small scale eddies and which is represented by an effective diffusivity. In chapter 3, we derive the fundamental solution of the equation and we show that the contours of the concentration of the tracer are a set of ellipsoids with principal axes changing with time according to the linear flow parameters and the diffusion. We then compute an apparent coefficient of diffusion that combines effects of the advection and diffusion and find that for short times, the eddy diffusion is dominant, and for large times, this coefficient depends on the parameters of the flow. In chapter 4, we illustrate the solution and the apparent coefficient of diffusion in case of simple linear flows and show how the growth of this coefficient varies. We expect our solution to be used to simulate the evolution of the concentration of a patch in realistic flows such that a non-linear flow by using a time stepping algorithm where we start by taking an initial Gaussian distribution and we assume that over a small time interval Δt, the velocity is assumed to be linear in space. The Gaussian solution obtained is now the initial condition for the restarted problem for the next time step. The error resulting from the linear approximation of the mean velocity field depends on the size of the principal axes of the patch. In case of large errors, the patch is divided into smaller patches.

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A Expressions for the constants in the time coefficients

$$
\begin{aligned}
C_x^1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{B''}{2\gamma^2 M(M-\gamma^2)} + \frac{(M-17\gamma^2)Q'^2-(M^2-3M\gamma^2+18\gamma^4)P'^2+2\gamma(M+15\gamma^2)P'Q'}{4\gamma^2(M-\gamma^2)^2S^2}\\
C_x^2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{Q'^2-MP'^2}{\gamma^2 M(M-\gamma^2)S} + \frac{2\eta_{xy}(h_{xy}+\eta_{xy})}{\gamma^2 M}\\
C_x^3(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{8(Q'-\gamma P')^2}{(M-\gamma^2)^2S^2}\\
C_x^4(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-8(Q'-\gamma P')(\gamma Q'-MP')}{(M-\gamma^2)^2S^2}\\
C_x^5(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-B}{2\gamma M(M-\gamma^2)} + \frac{-\gamma(7M+9\gamma^2)(Q'^2+MP'^2)+2M(M+15\gamma^2)P'Q'}{4\gamma M(M-\gamma^2)^2S^2}\\
C_x^6(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{B'}{2\gamma(M-\gamma^2)} + \frac{(M+15\gamma^2)(Q'^2+MP'^2)-2\gamma(7M+9\gamma^2)P'Q'}{4\gamma(M-\gamma^2)^2S^2}\\
C_x^7(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-\gamma(Q'^2+MP'^2)-2MP'Q'}{4\gamma M(M-\gamma^2)S^2} + \frac{B}{2\gamma M(M-\gamma^2)}\\
C_x^8(\alpha,\beta,\vec{h},\vec{\eta})) &= \frac{-(Q'^2+MP'^2)-2\gamma P'Q'}{4\gamma(M-\gamma^2)S^2} - \frac{B'}{2\gamma(M-\gamma^2)}\\
C_x^9(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-Q'^2+MP'^2}{4\gamma^2 MS^2} - \frac{2\eta_{xy}(h_{xy}+\eta_{xy})}{\gamma^2 M}\\
C_x^{10}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-B''}{2M\gamma^2(M-\gamma^2)} + \frac{-Q'^2+(M-2\gamma^2)P'^2-2\gamma P'Q'}{4\gamma^2(M-\gamma^2)S^2}
\end{aligned}
\tag{A.1}
$$

$$
\begin{aligned}
C_y^1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{A''}{2\gamma^2 M(M-\gamma^2)} + \frac{(M-17\gamma^2)Q^2 - (M^2-3M\gamma^2+18\gamma^4)P^2 + 2\gamma(M+15\gamma^2)PQ}{4\gamma^2(M-\gamma^2)^2 S^2} \\
C_y^2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{Q^2 - MP^2}{\gamma^2 M(M-\gamma^2)S} - \frac{2\eta_{xy}(h_{xy}-\eta_{xy})}{\gamma^2 M} \\
C_y^3(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{8(Q-\gamma P)^2}{(M-\gamma^2)^2 S^2} \\
C_y^4(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-8(Q-\gamma P)(\gamma Q - MP)}{(M-\gamma^2)^2 S^2} \\
C_y^5(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-A}{2\gamma M(M-\gamma^2)} + \frac{-\gamma(7M+9\gamma^2)(Q^2+MP^2) + 2M(M+15\gamma^2)PQ}{4\gamma M(M-\gamma^2)^2 S^2} \\
C_y^6(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{A'}{2\gamma(M-\gamma^2)} + \frac{(M+15\gamma^2)(Q^2+MP^2) - 2\gamma(7M+9\gamma^2)PQ}{4\gamma(M-\gamma^2)^2 S^2} \\
C_y^7(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-\gamma(Q^2+MP^2) - 2MPQ}{4\gamma M(M-\gamma^2)S^2} + \frac{A}{2\gamma M(M-\gamma^2)} \\
C_y^8(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(Q^2+MP^2) - 2\gamma PQ}{4\gamma(M-\gamma^2)S^2} - \frac{A'}{2\gamma(M-\gamma^2)} \\
C_y^9(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-Q^2+MP^2}{4\gamma^2 M S^2} + \frac{2\eta_{xy}(h_{xy}-\eta_{xy})}{\gamma^2 M} \\
C_y^{10}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-A''}{2M\gamma^2(M-\gamma^2)} + \frac{-Q^2 + (M-2\gamma^2)P^2 - 2\gamma PQ}{4\gamma^2(M-\gamma^2)S^2}
\end{aligned}
\tag{A.2}
$$

$$
\begin{aligned}
C_z^1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{A''(Q'^2+9\gamma^2P'^2-6\gamma P'Q')+B''(Q^2+9\gamma^2P^2-6\gamma PQ)+}{2\gamma^2M(M-\gamma^2)^2S^2} \\
&+\frac{2MC''(QQ'+9\gamma^2PP'-3\gamma(PQ'+P'Q))}{2\gamma^2M(M-\gamma^2)^2S^2}+\frac{AB-C^2}{M^2(M-\gamma^2)^2}-\frac{4\eta_{xy}^2}{\gamma^2M} \\
C_z^2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)^2}{\gamma^2M(M-\gamma^2)S^3}+\frac{\eta_{xy}(PQ'-P'Q)}{\gamma^2MS^2} \\
C_z^3(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{4(PQ'-P'Q)^2}{(M-\gamma^2)^2S^4}-\frac{4P'^2(A''+MA')+4P^2(B''+MB')+8PP'(MC''+MC')}{M(M-\gamma^2)^2S^2} \\
C_z^4(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{2(M-3\gamma^2)(PQ'-P'Q)^2}{\gamma(M-\gamma^2)^2S^4}+\frac{4P'^2(\gamma^2A'+A'')+4P^2(\gamma^2B'+B'')+8PP'(\gamma^2C'+MC'')}{\gamma(M-\gamma^2)^2S^2} \\
C_z^5(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(7M+9\gamma^2)(PQ'-P'Q)^2}{4M(M-\gamma^2)^2S^4}-\frac{P^2B+P'^2A+2PP'C}{2\gamma M(M-\gamma^2)S^2} \\
C_z^6(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(M+15\gamma^2)(PQ'-P'Q)^2}{4\gamma(M-\gamma^2)^2S^4}+\frac{P^2B'+P'^2A'+2PP'C'}{2\gamma(M-\gamma^2)S^2} \\
C_z^7(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{((M+11\gamma^2)A-4\gamma MA')P'^2+((M+11\gamma^2)B-4\gamma MB')P^2}{2\gamma M(M-\gamma^2)^2S^2} \\
&+\frac{2((M+11\gamma^2)C-4\gamma MC')PP'}{2\gamma M(M-\gamma^2)^2S^2}-\frac{\gamma(7M+9\gamma^2)(PQ'-P'Q)^2}{4\gamma M(M-\gamma^2)^2S^4}+\frac{A''B+B''A-2MC''C}{\gamma M^2(M-\gamma^2)^2} \\
C_z^8(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-((M+7\gamma^2)A'-8\gamma A)P'^2-((M+7\gamma^2)B'-8\gamma B)P^2-2((M+7\gamma^2)C'-8\gamma C)PP'}{2\gamma(M-\gamma^2)^2S^2} \\
&-\frac{(M+15\gamma^2)(PQ'-P'Q)^2}{4\gamma(M-\gamma^2)^2S^4} \\
C_z^9(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{4(PQ'-P'Q)^2}{(M-\gamma^2)^2S^4}+\frac{4P'^2(A''+MA')+4P^2(B''+MB')+8PP'(MC''+MC')}{M(M-\gamma^2)^2S^2} \\
C_z^{10}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{4P'^2(\gamma^2A'-A''-2\gamma A)+4P^2(\gamma^2B'-B''-2\gamma B)+8PP'(\gamma^2C'-MC''-2\gamma C)}{\gamma(M-\gamma^2)^2S^2} \\
&-\frac{2(M-3\gamma^2)(PQ'-P'Q)^2}{\gamma(M-\gamma^2)^2S^4} \\
C_z^{11}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)^2}{\gamma^2M(M-\gamma^2)S^3}+\frac{4\eta_{xy}(PQ'-P'Q)}{\gamma^2M(M-\gamma^2)S}+\frac{8\eta_{xy}^2}{\gamma^2M}+\frac{(A''+\gamma A)P'^2+(B''+\gamma B)P^2}{\gamma^2M(M-\gamma^2)S^2} \\
&+\frac{2(MC''+\gamma C)PP'}{\gamma^2M(M-\gamma^2)S^2} \\
C_z^{12}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(PQ'-P'Q)^2}{4\gamma^2(M-\gamma^2)S^4}+\frac{A''B''-M^2C''^2}{\gamma^2M^2(M-\gamma^2)^2}-\frac{((M-\gamma^2)A''+\gamma M(A+\gamma A'))P'^2}{\gamma^2M(M-\gamma^2)^2S^2} \\
&-\frac{((M-\gamma^2)B''+\gamma M(B+\gamma B'))P^2+2((M-\gamma^2)MC'+\gamma M(C+\gamma C'))PP'}{\gamma^2M(M-\gamma^2)^2S^2} \\
C_z^{13}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(PQ'-P'Q)^2}{4\gamma^2(M-\gamma^2)S^4}+\frac{-A''P'^2-B''P^2-2MC''PP'}{2\gamma^2M(M-\gamma^2)S^2}
\end{aligned}
\tag{A.3}
$$

$$
\begin{aligned}
C^1_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(M-17\gamma^2)QQ' + (M^2-3M\gamma^2+18\gamma^4)PP' - \gamma(M+15\gamma^2)(PQ'+P'Q)}{2\gamma^2(M-\gamma^2)^2S^2} \\
&\quad + \frac{MC''}{\gamma^2 M(M-\gamma^2)} \\
C^2_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-2(QQ'-MPP')}{\gamma^2M(M-\gamma^2)S} + \frac{-2\eta_{xy}(\alpha-\beta)}{\gamma^2 M} \\
C^3_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-16(Q-\gamma P)(Q'-\gamma P')}{(M-\gamma^2)S^2} \\
C^4_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{16\gamma QQ' + 16\gamma MPP' - 8(M+\gamma^2)(PQ'+P'Q)}{(M-\gamma^2)^2S^2} \\
C^5_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-C}{\gamma M(M-\gamma^2)} + \frac{\gamma(7M+9\gamma^2)(QQ'+MPP') - M(M+15\gamma^2)(PQ'+P'Q)}{2\gamma M(M-\gamma^2)^2S^2} \\
C^6_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{C'}{\gamma(M-\gamma^2)} + \frac{-(M+15\gamma^2)(QQ'+MPP') + \gamma(7M+9\gamma^2)(PQ'+P'Q)}{2\gamma(M-\gamma^2)S^2} \\
C^7_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{\gamma(QQ'+MPP') + M(PQ'+P'Q)}{2\gamma M(M-\gamma^2)S^2} + \frac{C}{\gamma M(M-\gamma^2)} \\
C^8_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(QQ'+MPP') + \gamma(PQ'+P'Q)}{2\gamma(M-\gamma^2)S^2} - \frac{C'}{\gamma(M-\gamma^2)} \\
C^9_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(QQ'-MPP')}{2\gamma^2MS^2} + \frac{2\eta_{xy}(\alpha-\beta)}{\gamma^2M} \\
C^{10}_{xy}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-MC''}{M\gamma^2(M-\gamma^2)} + \frac{QQ' - (M-2\gamma^2)PP' + \gamma(PQ'+P'Q)}{2\gamma^2(M-\gamma^2)S^2}
\end{aligned}
\tag{A.4}
$$

$$
\begin{aligned}
C^{1}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{((M+3\gamma^2)P'-4\gamma Q')A''+((M+3\gamma^2)P-4\gamma Q)MC''}{M\gamma^2(M-\gamma^2)^2S} \\
&\quad - \frac{2(Q-3\gamma P)(PQ'-P'Q)}{\gamma^2(M-\gamma^2)^2S^2} \\
C^{2}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-2Q(PQ'-P'Q)}{M\gamma^2(M-\gamma^2)S^2}+\frac{-2\eta_{xy}Q}{\gamma^2MS} \\
C^{3}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)(-12\gamma Q-2(M-11\gamma^2)P)}{\gamma(M-\gamma^2)^2S^3}+\frac{4(Q-\gamma P)MC''+4(Q'-\gamma P')A''}{\gamma M(M-\gamma^2)^2S} \\
C^{4}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)(2(-M+7\gamma^2)Q-4\gamma(2M+3\gamma^2)P)}{\gamma(M-\gamma^2)^2S^3}-\frac{4(\gamma Q-MP)MC''+4(\gamma Q'-MP')A''}{\gamma M(M-\gamma^2)^2S} \\
C^{5}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(-M(M+15\gamma^2)P+\gamma(7M+9\gamma^2)Q)(PQ'-P'Q)}{2\gamma M(M-\gamma^2)^2S^3}+\frac{PC+P'A}{\gamma M(M-\gamma^2)S} \\
C^{6}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(-(M+15\gamma^2)Q+\gamma(7M+9\gamma^2)P)(PQ'-P'Q)}{2\gamma(M-\gamma^2)^2S^3}+\frac{PC'+P'A'}{\gamma(M-\gamma^2)S} \\
C^{7}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(\gamma(5M+3\gamma^2)Q+(M+7\gamma^2)MP)(PQ'-P'Q)}{2\gamma M(M-\gamma^2)^2S^3} \\
&\quad + \frac{((M+3\gamma^2)A-4\gamma MA')P'+((M+3\gamma^2)C-4\gamma MC')P}{\gamma M(M-\gamma^2)^2S} \\
C^{8}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{((M+7\gamma^2)Q+\gamma(5M+3\gamma^2)P)(PQ'-P'Q)}{2\gamma(M-\gamma^2)^2S^3} \\
&\quad + \frac{(-(M+3\gamma^2)A'+4\gamma A)P'+(-(M+3\gamma^2)C'+4\gamma C)P}{\gamma(M-\gamma^2)^2S} \\
C^{9}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)(-4\gamma Q+2(M-3\gamma^2)P)}{\gamma(M-\gamma^2)^2S^3}+\frac{4(\gamma P-Q)MC''+4(\gamma P'-Q')A''}{\gamma M(M-\gamma^2)^2S} \\
C^{10}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(P'Q-PQ')(2(M-3\gamma^2)Q-4\gamma MP)}{2M\gamma^2(M-\gamma^2)S^3}+\frac{4\gamma(\gamma P'-Q')A'+4(\gamma P-Q)(\gamma C'-2\eta_{xy}(M-\gamma^2))}{\gamma(M-\gamma^2)^2S} \\
C^{11}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(P'Q-PQ')(-4\gamma MP+(M+3\gamma^2)Q)}{2M\gamma^2(M-\gamma^2)S^3}+\frac{2\eta_{xy}((M+3\gamma^2)Q-4\gamma MP)}{M\gamma^2(M-\gamma^2)S} \\
C^{12}_{yz}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)(Q+\gamma P)}{2\gamma^2(M-\gamma^2)S^3}+\frac{-P'A''-PMC''}{\gamma^2M(M-\gamma^2)S}
\end{aligned}
\tag{A.5}
$$

$$C_{xz}^{1}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{2(Q'-3\gamma P')(PQ'-P'Q)}{\gamma^2(M-\gamma^2)^2 S^2} + \frac{((M+3\gamma^2)P'-4\gamma Q')MC''+((M+3\gamma^2)P-4\gamma Q)B''}{M\gamma^2(M-\gamma^2)^2 S}$$

$$C_{xz}^{2}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{2Q'(PQ'-P'Q)}{M\gamma^2(M-\gamma^2)S^2} + \frac{2\eta_{xy}Q'}{\gamma^2 MS}$$

$$C_{xz}^{3}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{(PQ'-P'Q)(12\gamma Q'+2(M-11\gamma^2)P')}{\gamma(M-\gamma^2)^2 S^3} + \frac{4(Q-\gamma P)B''+4(Q'-\gamma P')MC''}{\gamma M(M-\gamma^2)^2 S}$$

$$C_{xz}^{4}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{(PQ'-P'Q)(2(M-7\gamma^2)Q'+4\gamma(2M+3\gamma^2)P')}{\gamma(M-\gamma^2)^2 S^3} - \frac{4(\gamma Q-MP)B''+4(\gamma Q'-MP')MC''}{\gamma M(M-\gamma^2)^2 S}$$

$$C_{xz}^{5}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{(M(M+15\gamma^2)P'-\gamma(7M+9\gamma^2)Q')(PQ'-P'Q)}{2\gamma M(M-\gamma^2)^2 S^3} - \frac{PB+P'C}{\gamma M(M-\gamma^2)S}$$

$$C_{xz}^{6}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{((M+15\gamma^2)Q'-\gamma(7M+9\gamma^2)P')(PQ'-P'Q)}{2\gamma(M-\gamma^2)^2 S^3} + \frac{PB'+P'C'}{\gamma(M-\gamma^2)S}$$

$$\begin{aligned} C_{xz}^{7}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{-(\gamma(5M+3\gamma^2)Q'+(M+7\gamma^2)MP')(PQ'-P'Q)}{2\gamma M(M-\gamma^2)^2 S^3} \\ &+ \frac{((M+3\gamma^2)B-4\gamma MB')P+((M+3\gamma^2)C-4\gamma MC')P'}{\gamma M(M-\gamma^2)^2 S} \end{aligned}$$

$$\begin{aligned} C_{xz}^{8}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(-(M+7\gamma^2)Q'-\gamma(5M+3\gamma^2)P')(PQ'-P'Q)}{2\gamma(M-\gamma^2)^2 S^3} \\ &+ \frac{(-(M+3\gamma^2)B'+4\gamma B)P+(-(M+3\gamma^2)C'+4\gamma C)P'}{\gamma(M-\gamma^2)^2 S} \end{aligned}$$

$$C_{xz}^{9}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{(PQ'-P'Q)(4\gamma Q'-2(M-3\gamma^2)P')}{\gamma(M-\gamma^2)^2 S^3} + \frac{4(\gamma P-Q)B''+4(\gamma P'-Q')MC''}{\gamma M(M-\gamma^2)^2 S}$$

$$\begin{aligned} C_{xz}^{10}(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)(-2(M-3\gamma^2)Q'+4\gamma MP')}{\gamma(M-\gamma^2)^2 S^3} \\ &+ \frac{4\gamma(\gamma P-Q)B'+4(\gamma P'-Q')(\gamma C'+2\eta_{xy}(M-\gamma^2)(\gamma P'-Q')}{\gamma(M-\gamma^2)^2 S} \end{aligned}$$

$$C_{xz}^{11}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{(P'Q-PQ')(4\gamma MP'-(M+3\gamma^2)Q')}{2M\gamma^2(M-\gamma^2)S^3} + \frac{2\eta_{xy}(-(M+3\gamma^2)Q'+4\gamma MP')}{M\gamma^2(M-\gamma^2)S}$$

$$C_{xz}^{12}(\alpha,\beta,\vec{h},\vec{\eta}) = \frac{-(PQ'-P'Q)(Q'+\gamma P')}{2\gamma^2(M-\gamma^2)S^3} + \frac{-PB''-P'MC''}{\gamma^2 M(M-\gamma^2)S} \tag{A.6}$$

$$
\begin{aligned}
R_1(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{8((M-\gamma^2)A'' + 2\gamma MA - 2M\gamma^2 A')P'^2 + 8((M-\gamma^2)B'' + 2\gamma MB - 2M\gamma^2 B')P^2}{\gamma M(M-\gamma^2)^3 S^2} \\
&\quad + \frac{16((M-\gamma^2)MC'' + 2\gamma MC - 2M\gamma^2 C')PP'}{\gamma M(M-\gamma^2)^3 S^2} + \frac{4(M-5\gamma^2)(PQ'-P'Q)^2}{\gamma(M-\gamma^2)^3 S^4} \\
R_2(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(-\gamma(3M+5\gamma^2)A + M(M+7\gamma^2)A')P'^2 + (-\gamma(3M+5\gamma^2)B + M(M+7\gamma^2)B')P^2}{\gamma M(M-\gamma^2)^3 S^2} \\
&\quad + \frac{2(-\gamma(3M+5\gamma^2)C + M(M+7\gamma^2)C')PP'}{\gamma M(M-\gamma^2)^3 S^2} + \frac{(M^2 + 22M\gamma^2 + 9\gamma^4))(PQ'-P'Q)^2}{4\gamma M(M-\gamma^2)^3 S^4} \\
&\quad - \frac{AB - C^2}{\gamma M^2 (M-\gamma^2)^2} \\
R_3(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(8\gamma A - 4(M+\gamma^2)A')P'^2 + (8\gamma B - 4(M+\gamma^2)B')P^2 + 2(8\gamma C - 4(M+\gamma^2)C')PP'}{(M-\gamma^2)^3 S^2} \\
&\quad - \frac{(2(M+3\gamma^2)(PQ'-P'Q)^2}{(M-\gamma^2)^3 S^4} \\
R_4(\alpha,\beta,\vec{h},\vec{\eta}) &= \frac{(PQ'-P'Q)^2}{\gamma^3 M(M-\gamma^2)S^3} + \frac{4\eta_{xy}(PQ'-P'Q)}{\gamma^3 M(M-\gamma^2)S} + \frac{4\eta_{xy}^2}{\gamma^3 M} + \frac{\eta_{xy}(PQ'-P'Q)}{\gamma^3 M S^2} \\
R_5(\alpha,\beta,\vec{h},\vec{\eta}) &= -\frac{((M-\gamma^2)A'' + \gamma M(A+\gamma A'))P'^2 + ((M-\gamma^2)B'' + \gamma M(B+\gamma B'))P^2}{2\gamma^3 M(M-\gamma^2)^2 S^2} \\
&\quad - \frac{2((M-\gamma^2)MC' + \gamma M(C+\gamma C'))PP'}{2\gamma^3 M(M-\gamma^2)^2 S^2} - \frac{M^2 C''^2 - A''B''}{2\gamma^3 M^2 (M-\gamma^2)^2} - \frac{(PQ'-P'Q)^2}{8\gamma^3 (M-\gamma^2) S^4}
\end{aligned}
\tag{A.7}
$$