Analytical Gaussian Solutions for Anisotropic Diffusion in a Linear Shear Flow

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Communicated by J. Schröter, Paderborn, Germany
Registration Number 657

Abstract
An extended diffusion equation is derived which takes into account anisotropic transport of mass in a shear flow. Analytical solutions for systems with spatially linear but time-dependent flow and sedimentation velocities, a time-dependent diffusion tensor as well as linear sinks and sources are determined. Considering only systems in spatially infinite domains, the solutions for Gaussian initial distributions are derived. Then, starting from this general case, the two- and three-dimensional solutions are deduced for a horizontal and linear shear flow which generalize the results of former Gaussian plume models. Further, it is shown that the extended diffusion equation can be treated by solution methods of the Fokker-Planck equation. Finally, it is discussed how the time-dependent diffusion tensor can be determined from the first and second moments of these solutions.

1. Introduction
It is a well-known fact that under suitable conditions, which normally amount to a requirement that the Reynolds number be sufficiently large, the macroscopic velocity of the considered fluid takes "random values" for which only average properties can be uniquely determined in terms of measurable quantities. Fluctuating motions of this kind are said to be turbulent. Transport of mass caused by these motions is usually denoted as a turbulent transport or turbulent diffusion.

Turbulent diffusion, although subject of a long-lasting research history, recently gains growing importance in the community of environmental studies. For example, airtraffic increased significantly in the past (approximately 5% per year) and is expected to increase in future. The resulting increase of pollution emissions from the aircraft engines, especially at the cruising height of about 10 km, gives rise to the concern of a possible impact of such emissions on the state of the atmosphere and the earth's climate [1].
At cruising altitude, the atmospheric mean flow is dominated by its horizontal component. Additionally, the regions of strong wind shear and resulting turbulence are observed at these heights [2]. The vertical stability of the upper troposphere and stratosphere is characterized by a fast decay of vertical flow fluctuations. This is a consequence of the stable stratification of the air density due to its decrease with the height. According to these properties, such flows are usually denoted as stably stratified shear flows. In the ocean, which also is stably stratified and sheared, the mixing processes of momentum, heat, and species concentrations are still poorly understood [3]. Therefore, it is desirable to develop theoretical tools describing mixing and dispersion processes in turbulent environments which are both sheared and stably stratified.

Starting from an appropriately generalized diffusion equation, the dispersion of arbitrary species in a sheared flow is considered in this paper. The dispersion includes effects due to advection, gravitational sedimentation, anisotropic diffusion, and (linear) chemical reactions. We discuss an initial value problem in spatially infinite domain with sources characterized by three-dimensional Gaussian distribution functions. Additionally, the validity of Fick’s law is assumed as a closing relation for the diffusion flux. It is well-known that the transport properties of mass in a sheared flow are strongly anisotropic [4]. This is the consequence of turbulent fluctuations of the velocity flow forced by shear of the considered mean flow and buoyancy. Due to that anisotropy of turbulence, all components of the diffusion tensor have to be taken into account which, generally, also depend on time [5, 6].

The diffusion equation reduces under some assumptions to the well-known Fokker-Planck equation. Therefore, the solution methods developed within this framework [7, 8] can be applied. The analytical solutions obtained in this paper generalize the results of the Gaussian plume models [9–13] in such a way that both the complete, time-dependent diffusion tensor and an arbitrary shear flow with a spatially constant but time-dependent shear matrix are taken into account. Additionally, a time-dependent sedimentation velocity together with linear chemical reactions are considered.

These solutions are useful for the following two goals: First, one obtains a practicable prescription how an appropriate diffusion tensor can be determined from the first and second moments of the measured or simulated density of a tracer undergoing diffusion in a stably stratified flow. Second, this kind of solutions can be directly applied for the modelling of dispersion for the typical sources of pollution as point and line sources. For example, the two-dimensional solution which will be discussed in this paper was recently used to estimate the increase of nitrogen oxides (which are relevant in the chemistry of atmospheric ozone) caused by the airtraffic over the North Atlantic [14].

In Section 2, we specify and solve the extended diffusion equation. This solution is applied in Section 3 to conditions of a horizontal and linear shear flow. In Section 4 the obtained results are shortly discussed.
2. Extended diffusion equation

We start with a system of classical balances of mass for a mixture including \( M \) different species with densities \( \rho_\alpha, \alpha = 1, \ldots, M \) (in kg/m\(^3\)). The balance equations read

\[
\partial_t \rho_\alpha(x, t) + \nabla_x \cdot \mathbf{j}_\alpha(x, t) = Q_\alpha(x, t)
\]

(1)

with

\[
\alpha = 1, \ldots, M \quad x \in \Omega \subset \mathbb{R}^3, \quad t \in \mathbb{R}^+.
\]

where \( \mathbf{j}_\alpha \) and \( Q_\alpha \) denote the mass flux (in kg/m\(^2\)s) and the sources (or sinks) (in kg/m\(^2\)s) of the \( \alpha \)-species. In order to obtain a system of equations from which the densities \( \rho_\alpha \) can be determined, one has to express \( \mathbf{j}_\alpha \) and \( Q_\alpha \) in terms of the densities \( \rho_\alpha \) (so-called closing relations). In addition, proper initial and boundary conditions are needed. The aim of the following assumption is twofold. First, the closing relations should be formulated in such a way that the most important properties of a shear flow in spatially infinite domain are taken into account. Second, we are interested in analytical solutions of (1) which can only be obtained under some limiting assumptions.

**Assumption 2.1**

1. We devide the flux \( \mathbf{j}_\alpha \) in three subfluxes

\[
\mathbf{j}_\alpha := \mathbf{j}_{u\alpha} + \mathbf{j}_{s\alpha} + \mathbf{j}_{D\alpha},
\]

(2)

where the subscripts \( u, s, \) and \( D \) denote the flux caused by the advection with the flow velocity \( \mathbf{u} \) of the background continuum, the sedimentation flux due to the gravitation and the diffusion flux of the considered \( \alpha \)-species, respectively. Especially, using the notation of coordinates introduced in Figure 1, we assume for the subfluxes

\[
\mathbf{j}_{u\alpha}(x, t) := \rho_\alpha(x, t) \mathbf{u}(x, t),
\]

(3)

\[
\mathbf{j}_{s\alpha}(x, t) := \kappa(x, t) \rho_\alpha(x, t) \mathbf{g},
\]

(4)

\[
\mathbf{j}_{D\alpha}(x, t) := - \mathbf{D}(t) \cdot \nabla_x \rho_\alpha(x, t),
\]

(5)

![Diagram](image)

**Fig. 1:** Definition of the used coordinate system.
where the function \( \kappa \) (in s) describes sedimentation properties of the background flow and \( D \) (in m\(^2\)/s) denotes a symmetric and positive-definite diffusion tensor (Fick’s law). In the following, only a linear dependence of \( u \) and \( \kappa \) from the space coordinate \( x \) is considered, i.e.,

\[
\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_0(t) + \mathbf{s}(t) \cdot \mathbf{x},
\]

\[
\kappa(\mathbf{x}, t) = \kappa_0(t) + \kappa_s(t) x_3
\]

where \( \mathbf{u}_0 \) is the space-independent part of \( \mathbf{u} \) and \( \mathbf{s} \) denotes the time-dependent 3 \( \times \) 3 shear matrix. Similarly, \( \kappa_0 \) and \( \kappa_s \) are time-dependent functions.

2. For the modelling of sources and sinks of equation (1), only linear chemical reactions are taken into account, i.e.,

\[
Q_\alpha(\mathbf{x}, t) = - \sum_{\beta=1}^{M} r_{\alpha\beta}(t) \rho_\beta(\mathbf{x}, t),
\]

where \( (r_{\alpha\beta}), \alpha, \beta = 1, \ldots, M \) denotes a \( M \times M \) matrix of the time-dependent reaction coefficients (in s\(^{-1}\)).

3. The initial conditions for \( \rho_\alpha \) are described by three-dimensional Gaussian functions defined in (32) (see appendix), i.e.,

\[
\rho_{0\alpha}(\mathbf{x}) := \rho_\alpha(\mathbf{x}, 0) = c_\alpha \varphi(\mathbf{x}, \bar{x}_0, \sigma_0)
\]

\[
:= c_\alpha (2\pi)^{-3/2}(\det \sigma_0)^{-1/2} \exp \left[ -\frac{1}{2}(\mathbf{x} - \bar{x}_0) \cdot \sigma_0^{-1} (\mathbf{x} - \bar{x}_0) \right].
\]

Here, \( \bar{x}_0 \) denotes the mean value and \( \sigma_0 \) the variance matrix of \( \varphi \) (in m\(^2\)). The total initial mass of the \( \alpha \)-species is \( c_\alpha \) (in kg).

4. We confine our further discussion to problems in a spatially infinite domain. This means for domain \( \Omega \) of (1) that \( \Omega = \mathbb{R}^3 \times \mathbb{R}^+ \). Additionally, the solutions of (1) have to satisfy the conditions

\[
\lim_{|\mathbf{x}| \to \infty} \rho_\alpha(\mathbf{x}, t) = 0, \quad \forall t \in \mathbb{R}^+, \quad \alpha = 1, \ldots, M.
\]

**Conclusion**

Starting from (1) together with the proposed assumption 2.1, one obtains the following equations for the densities \( \rho_\alpha \)

\[
[\partial_t + a_i(t)\partial_{x_i} - A_{ij}(t)\partial_{x_i}x_j - D_{ij}(t)\partial_{x_i}\partial_{x_j}] \rho_\alpha(\mathbf{x}, t) + \sum_{\beta=1}^{M} r_{\alpha\beta}(t) \rho_\beta(\mathbf{x}, t) = 0
\]

with
\[ a(t) = \begin{pmatrix} u_{01}(t) \\ u_{02}(t) \\ u_{03}(t) - \kappa_0(t)g \end{pmatrix}, \quad A(t) = \begin{pmatrix} s_{11}(t) & s_{12}(t) & s_{13}(t) \\ s_{21}(t) & s_{22}(t) & s_{23}(t) \\ s_{31}(t) & s_{32}(t) & s_{33}(t) - \kappa_s(t)g \end{pmatrix} \]

and the initial conditions
\[ \rho_{0\alpha}(x) = c_\alpha \varphi(x, \bar{x}_0, \sigma_0), \quad \alpha = 1, \ldots, M. \] (12)

Due to the fact that the system of partial differential equations given by (11) and (12) can be understood as an extension of the usual diffusion equation, the notation extended diffusion equation will be used. Furthermore, although the turbulent diffusion tensor is generally non-symmetric [6], only its symmetric part is relevant in the extended diffusion equation (11). Consequently, the required symmetry of D does not confine the possible solutions of (11). Finally, equation (11) reduces for \( a = 0 \) and \( r_{\alpha\beta} = 0, \alpha, \beta = 1, \ldots, M \) to the well-known Fokker-Planck equation for the Ornstein-Uhlenbeck process [15]. This kind of equation is also known as the Smoluchowski equation with a linear force [16]. Therefore, one expects that the methods of solutions developed within this framework can also be applied in the case of the extended diffusion equation (11).

**Proposition 2.2**

The solution of the system (11) satisfying condition (10) together with the initial conditions (12) can be written in the form
\[ \rho_\alpha(x,t) = f_\alpha(t) \varphi(x, \bar{x}(t), \sigma(t)), \quad \alpha = 1, \ldots, M, \] (13)

where \( \varphi \) is the three-dimensional Gaussian function defined by (9) and the functions \( f_\alpha \) satisfy the system of ordinary differential equations given by
\[ \frac{df_\alpha(t)}{dt} + \sum_{\beta=1}^{M} r_{\alpha\beta}(t) f_\beta(t) = 0, \quad f_\alpha(0) = c_\alpha. \] (14)

In order to obtain the parameters of (13), the mean value \( \bar{x} \) and the variance matrix \( \sigma \), one has to solve two systems of ordinary differential equations which read
\[ \frac{d\bar{x}(t)}{dt} = -A(t) \cdot \bar{x}(t) + a(t), \quad \bar{x}(0) = \bar{x}_0 \] (15)

and
\[ \frac{d\sigma(t)}{dt} = -A(t) \cdot \sigma(t) - [A(t) \cdot \sigma(t)]^T + 2D(t), \quad \sigma(0) = \sigma_0. \] (16)
Analytical Gaussian solutions for anisotropic diffusion

Proof:
To solve system (11) we use the transformation given by

$$\rho_\alpha(x, t) = f_\alpha(t) g_\alpha(x, t) \quad \alpha = 1, \ldots, M,$$  \hspace{1cm} (a)

where functions $f_\alpha$ are defined as the solutions of (14) which, under some weak assumptions for the matrix $(r_{\alpha\beta})$, are unique. According to the initial conditions (9), the relations

$$g_\alpha(x, 0) = \varphi(x, \bar{x}_0, \sigma_0)$$  \hspace{1cm} (b)

have to be fulfilled. Inserting (a) into (11) yields a system of equations given by

$$0 = f_\alpha^{-1}(t) \left[ \frac{df_\alpha(t)}{dt} + \sum_{\beta=1}^{M} r_{\alpha\beta}(t) f_\beta(t) \right]$$

$$= g_\alpha^{-1}(x, t) \left[ \partial_t + a_\alpha(t) \partial_{x_\alpha} - A_{ij}(t) \partial_{x_i} x_j - D_{ij}(t) \partial_{x_i} \partial_{x_j} \right] g_\alpha(x, t).$$

Assuming $g_\alpha \neq 0$, one obtains

$$\left[ \partial_t + a_\alpha(t) \partial_{x_\alpha} - A_{ij}(t) \partial_{x_i} x_j - D_{ij}(t) \partial_{x_i} \partial_{x_j} \right] g_\alpha(x, t) = 0.$$  \hspace{1cm} (c)

For $\alpha = 0$ and $M = 1$, equation (c) reduces to the well-known Fokker-Planck equation for the Ornstein-Uhlenbeck process [15]. Using the methods of solution described in [7] and [8] the ansatz

$$g_\alpha(x, t) = \varphi(x, \bar{x}(t), \sigma(t))$$

leads to general solutions of (c). Here, $\bar{x}$ and $\sigma$ are arbitrary functions solely depending on time and satisfying the initial conditions

$$\bar{x}(0) = \bar{x}_0, \quad \sigma(0) = \sigma_0.$$

With the help of relation (36) (see appendix), the three-dimensional Gaussian function $\varphi$ can be transformed to

$$\hat{\varphi}(k, \bar{x}(t), \sigma(t)) := \mathcal{F} \left[ \varphi(\cdot, \bar{x}(t), \sigma(t)) \right](k)$$

$$= (2\pi)^{-3/2} \int_{\mathbb{R}^3} \varphi(x, \bar{x}(t), \sigma(t)) \exp(i k \cdot x) \, dx$$

$$= (2\pi)^{-3/2} \exp \left[ i k \cdot \bar{x}(t) - \frac{1}{2} k \cdot \sigma(t) \cdot k \right].$$  \hspace{1cm} (d)

Making use of the Gauß theorem, the Fourier transformation of (c) yields

$$\left[ \partial_t - ia_\alpha(t) k_\alpha + A_{ij}(t) k_i \partial_{k_j} + D_{ij}(t) k_i k_j \right] \phi(k, \bar{x}(t), \sigma(t)) = 0.$$  \hspace{1cm} (e)

Inserting the Fourier transform (d) into (e) and carrying out all the derivatives leads to a polynomial in $k$ for $k \in \mathbb{R}^3$. Consequently, the coefficients of this polynomial must vanish, which immediately leads to the systems of equations (15) and (16). Due to the fact that $D$ and $\sigma_0$ are symmetric and positive-definite, the solution of (16) has the same properties [7]. Therefore, the solutions (13) satisfy all the conditions (10).

Consequences 2.3

1. Equations (14), (15), and (16) can be solved making use of the known methods of solutions for systems of ordinary and linear differential equations (see, e.g., [17]). In the case that the matrix $(r_{\alpha\beta})$ does not depend on time, the solutions of (14) can be expressed in terms of the Laplace transformation,

$$f_\alpha(t) = \sum_{\beta=1}^{M} \mathcal{L}^{-1}[\tilde{f}_{\alpha\beta}^{-1}(\cdot)](t)c_\beta,$$

where the matrix $(\tilde{r}_{\alpha\beta})$ is defined by

$$\tilde{r}_{\alpha\beta}: \mathbb{R} \to \mathbb{R}, \ s \to \tilde{r}_{\alpha\beta}(s):= s \delta_{\alpha\beta} + r_{\alpha\beta}$$

and $\mathcal{L}^{-1}$ denotes the inverse Laplace transformation.

2. According to [7], the variance matrix $\sigma$ can be calculated from

$$\sigma(t) = G(t,0) \cdot \sigma_0 \cdot G^T(t,0) + 2 \int_0^t G(t,t') \cdot D(t') \cdot G^T(t,t') \, dt'$$

where the evolution operator $G$ is defined by

$$\frac{dG(t,t')}{dt} = -A(t) \cdot G(t,t'), \quad G(t',t') = 1.$$  

(19)

The formal solution of (19) can be written as

$$G(t,t') = \exp -\tilde{A}(t,t') := 1 - \tilde{A} + \frac{1}{2} \tilde{A}^2 \pm \cdots$$

$$\tilde{A}(t,t') := \int_{t'}^t A(x) \, dx.$$  

(20)

In the case that $A$ does not depend on time, the matrix $\tilde{A}$ can be explicitly calculated. Then, one gets for the evolution operator $G$

$$G(t,t') = \exp -A(t-t') := 1 - A(t-t') + \frac{1}{2} A^2(t-t')^2 \pm \cdots.$$  

(21)

If $A$ is a nilpotent matrix with $A^k = 0$, then only the first $k$ terms of the series (21) do not vanish. The best known example of a nilpotent $3 \times 3$ matrix is a so-called strictly upper (or lower) triangular matrix ($A_{ij} = 0$ for $i \leq j$ (or $i \geq j$), $i, j = 1, \ldots, 3$) with $k = 3$. 

3. In the case that $A$ is independent of time, equation (15) can also be formally solved [17]. One obtains

$$\bar{x}(t) = G(t, 0) \cdot \bar{x}_0 + \int_0^t G(t, t') \cdot a(t') dt'$$

(22)

where $G$ is given by (21).

4. Due to the fact that the two lowest moments of the Gaussian function can be expressed in terms of the mean value $\bar{x}$ and the variance matrix $\sigma$ (see appendix, equations (34) and (35)), the following relations hold

$$E(\rho_\alpha) = \bar{x}, \quad \text{var}(\rho_\alpha) = \sigma, \quad \alpha = 1, \ldots, M$$

(23)

where $E(\rho_\alpha)$, $\text{var}(\rho_\alpha)$ denote the (normalized) mean value and variance matrix of the solution (13), respectively, which generally can be considered as measureable quantities. These quantities can be used for the following two goals: First, with the help of (13) a three-dimensional Gaussian functions $\bar{\rho}_\alpha$ defined by

$$\bar{\rho}_\alpha(x, t) := f_\alpha(t) \varphi(x, E(\cdot)(t), \text{var}(\cdot)(t)), \quad \alpha = 1, \ldots, M$$

(24)

can be introduced for the modelling of the measured concentrations because the lowest two moments of $\bar{\rho}_\alpha$ agree with the observed moments $E(\cdot)$ and $\text{var}(\cdot)$. Second, assuming the validity of the assumption 2.1 and taking into account relation (16), an appropriate diffusion tensor $D$ can be determined that can also be used for the description of diffusion occurring in arbitrary flows.

3. Explicit solutions for a horizontal and linear shear flow

In order to determine the solutions (13) explicitly, the ordinary systems of differential equations (14), (15), and (16) have to be solved. In most atmospheric and oceanographic applications, it is sufficient to restrict the general results of the previous section to (incompressible) fluids dominated by a horizontal velocity field.

Assumption 3.1

1. To describe a horizontal and linear shear flow, the following uniaxial, time-independent and linearly sheared velocity field is considered

$$\mathbf{u} = \begin{pmatrix} u_1(x_2, x_3) \\ 0 \\ 0 \end{pmatrix}, \quad u_1(x_2, x_3) = u_0 + s_2 x_2 + s_3 x_3$$

(25)

with $u_0$, $s_2$, $s_3 = \text{const}$. Here, $s_2$ and $s_3$ denote the horizontal and vertical shear, respectively.

2. Additionally, only a constant sedimentation velocity is taken into account, i.e., \( \kappa(\mathbf{x}, t) = \kappa_0 = \text{const} \).

**Remark 3.2**

In the case of an incompressible fluid, the uniaxial and linearly sheared flow described by

\[
\mathbf{u} = \begin{pmatrix} u_1(x_1, x_2, x_3) \\ 0 \\ 0 \end{pmatrix}, \quad u_1(x_1, x_2, x_3) = u_0 + s_1 x_1 + s_2 x_2 + s_3 x_3
\] (26)

is only possible for \( s_1 = 0 \). Consequently, one can justify neglecting of \( s_1 \) in (25) due to the fact that in most atmospheric and oceanographic applications only incompressible fluids are considered.

With the help of this assumption, equations (15) and (16) can be solved explicitly.

**Proposition 3.3**

1. The solution of (15) reads

\[
\bar{x}(t) = \begin{pmatrix} \bar{x}_{01} + (u_0 + s_2 \bar{x}_{02} + s_2 \bar{x}_{03}) t - \frac{1}{2} s_3 \kappa_0 g t^2 \\ \bar{x}_{02} \\ \bar{x}_{03} - \kappa_0 g t \end{pmatrix}.
\] (27)

2. The solution of (15) for the symmetric matrix \( \sigma \) can be written as follows:

\[
\sigma_{11}(t) = \sum_{k=0}^{2} (-1)^k \binom{2}{k} (s_2 \bar{D}^{(k)}_{22}(t) + 2 s_2 s_3 \bar{D}^{(k)}_{23}(t) + s_2 s_3 \bar{D}^{(k)}_{33}(t)) t^{2-k}
\]

\[
+ \bar{D}^{(0)}_{11}(t) + 2 \sum_{k=0}^{1} (-1)^k (s_2 \bar{D}^{(k)}_{12}(t) + s_3 \bar{D}^{(k)}_{13}(t)) t^{1-k},
\]

\[
\sigma_{12}(t) = \bar{D}^{(0)}_{12}(t) + \sum_{k=0}^{1} (-1)^k (s_2 \bar{D}^{(k)}_{22}(t) + s_3 \bar{D}^{(k)}_{23}(t)) t^{1-k},
\]

\[
\sigma_{13}(t) = \bar{D}^{(0)}_{13}(t) + \sum_{k=0}^{1} (-1)^k (s_2 \bar{D}^{(k)}_{22}(t) + s_3 \bar{D}^{(k)}_{23}(t)) t^{1-k},
\]

\[
\sigma_{22}(t) = \bar{D}^{(0)}_{22}(t), \quad \sigma_{23}(t) = \bar{D}^{(0)}_{23}(t), \quad \sigma_{33}(t) = \bar{D}^{(0)}_{33}(t)
\]

with

\[
\bar{D}^{(k)}_{ij}(t) := 2 \int_{0}^{t} x^k D_{ij}(x) dx + \delta_{k0} \sigma_{0ij}, \quad i, j = 1, \ldots, 3, \quad k \in \mathbb{N}_0.
\] (29)
Proof:
Starting from assumption 3.1, one gets
\[ a = \begin{pmatrix} u_0 \\ 0 \\ -\kappa_0 \theta \end{pmatrix}, \quad A = -\begin{pmatrix} 0 & s_2 & s_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]
for the vector \( a \) and the matrix \( A \). Since \( a \) and \( A \) do not depend on time, the system of equations (15) can easily be solved. Making use of (22), one obtains relation (18). Furthermore, the matrix \( A \) is nilpoint with \( A^2 = 0 \). Taking into account (21), one gets
\[ G(t, t') = \begin{pmatrix} 1 & s_2(t - t') & s_3(t - t') \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \]
According to the solution (18), straightforward algebraic calculations lead to formula (28).

Remarks 3.4
1. For a time-independent diffusion tensor \( D \), the moments (29) can be explicitly calculated. One obtains
\[ \bar{D}^{(k)}_{ij}(t) = \frac{2}{k+1} D_{ij} t^{k+1} + \delta_{k0} \sigma_{0ij}. \]  
(30)
Inserting (30) into (28) yields polynomials in \( t \) for the components of \( \sigma \). Especially, one gets a cubic polynomial for \( \sigma_{11} \) and quadratic polynomials for \( \sigma_{12} \) and \( \sigma_{13} \). The components \( \sigma_{22}, \sigma_{23} \) and \( \sigma_{33} \) are linear in \( t \). Consequently, if such a time-dependence of \( \sigma \) is experimentally observed (at least approximately), a time-independent diffusion tensor may be used for the modelling of the considered dispersion. Due to the fact that equations (28) are linear in \( D \), the particular components \( D_{ij} \) can be easily calculated.

2. For many relevant applications, the relation \( s_2 \ll s_3 \) holds, meaning that the horizontal shear is much smaller than the vertical ones. Consequently, \( s_2 \) can be neglected. In these cases, it is often sufficient to discuss a two-dimensional diffusion in the \( x_1-x_3 \)-plane. Then, the solution for a time-independent diffusion tensor can be written as
\[ \rho_\alpha(x, t) = f_\alpha(t) \varphi(x, \bar{x}(t), \sigma(t)), \quad \alpha = 1, \ldots, M \]
(31)
with
\[ x = \begin{pmatrix} x_1 \\ x_3 \end{pmatrix}, \quad \bar{x}(t) = \begin{pmatrix} \bar{x}_{01} + (u_0 + s_3 \bar{x}_{03}) t - \frac{1}{2} s_3 \kappa_0 g t^2 \\ \bar{x}_{03} - \kappa_0 g t \end{pmatrix}, \]
\[ \sigma(t) = \begin{pmatrix} \sigma_{11}(t) & \sigma_{13}(t) \\ \sigma_{13}(t) & \sigma_{33}(t) \end{pmatrix}, \]

and

\[ \sigma_{11}(t) = \frac{2}{3} s_3^2 D_{33} t^3 + (2 s_3 D_{13} + s_3^2 \sigma_{033}) t^2 + 2(s_3 \sigma_{013} + D_{11}) t + \sigma_{011}, \]

\[ \sigma_{13}(t) = s_3 D_{33} t^2 + (s_3 \sigma_{033} + 2 D_{13}) t + \sigma_{013}, \]

\[ \sigma_{33}(t) = 2 D_{33} t + \sigma_{033}. \]

Neglecting the sedimentation velocity \((\kappa_0 = 0)\), the chemical reactions \((r_{\alpha \beta} = 0, \alpha, \beta = 1, \ldots, M)\) and assuming \(D_{13} = 0\) together with \(\sigma_0 = 0\), one obtains the results given in [10], [11], and [13]. Additionally, for \(D := D_{11} = D_{33}\), one gets the well-known solution of a Gaussian plume model [12], i.e.,

\[ \rho(x_1, x_3, t) = \frac{c}{2 \pi \hat{\sigma}_h \hat{\sigma}_v} \exp \left[ - \left( \frac{(x_1 - \bar{x}_{01} - u_0 t - \frac{1}{2} s_3 x_3)^2}{2 \hat{\sigma}_h^2} + \frac{(x_3 - \bar{x}_{03})^2}{2 \hat{\sigma}_v^2} \right) \right] \]

with

\[ \hat{\sigma}_v^2 = 2 D t, \quad \hat{\sigma}_h^2 = 2 D t \left( 1 + \frac{1}{12} s_3^2 t^2 \right) \]

where only one species is considered.

4. Conclusions

Starting from the extended diffusion equation (11) derived in Section 2 and due to its similarity to the well-known Fokker-Planck equation for the Ornstein-Uhlenbeck process, the solutions of (11) were deduced. As a consequence of this approach, Gaussian solutions were obtained which generalize the corresponding results usually discussed within the framework of the fluid dynamics and atmospheric physics.

Furthermore, the obtained solutions were written down explicitly for a horizontal and linear shear flow. For example, in the case of a given time-dependent diffusion tensor \(\mathbf{D}\), one has to calculate the integrals (29) which together with (27), (28), and the solutions of (14) lead to the explicit solutions of the extended diffusion equation (11). Due to the fact that the derived solutions are Gaussian functions satisfying Gaussian initial conditions, one can use these solutions iteratively by taking into account different parameters in every step of such iteration.

Making use of equation (16) or (28), it is also possible to determine an appropriate time-dependent diffusion tensor from the variance matrix \(\boldsymbol{\sigma}\) that, generally, can be understood as a measurable quantity. For a time-independent diffusion tensor, one obtains from (28) explicit relations for the particular components of \(\mathbf{D}\) only in terms of the variance matrix \(\boldsymbol{\sigma}\).
Acknowledgments

This work was supported by BMFT within the research program "Schadstoffe in der Luftfahrt" (Pollution from Aviation). The author thanks U. Schumann and T. Gerz (DLR) for stimulating this research and helpful discussions. J. Schröter and R. Wegener (University of Paderborn) contributed to this work with useful comments.

A. Gaussian functions and their properties

The aim of this appendix is to collect the definition and all the properties of the $n$-dimensional Gaussian functions which are needed in this paper. For a complete presentation see [18], [19] and [20].

Definition A.1 (Gaussian functions)

Let $\bar{x} \in \mathbb{R}^n$ and $\sigma \in M_n(\mathbb{R})$ be a real, symmetric and positive-definite $n \times n$-matrix. Functions $\varphi(\cdot, \bar{x}, \sigma) : \mathbb{R}^n \rightarrow \mathbb{R}$ with

$$x \mapsto \varphi(x, \bar{x}, \sigma) = (2\pi)^{-n/2} (\det \sigma)^{-1/2} \exp \left[ -\frac{1}{2} (x - \bar{x}) \cdot \sigma^{-1} \cdot (x - \bar{x}) \right]$$  \hspace{1cm} (32)

are denoted as $n$-dimensional Gaussian functions.

Remarks A.2

1. $M_n(\mathbb{R})$ denotes the real $n \times n$-matrices.

2. The $n$-dimensional Gaussian functions satisfy the normalization condition

$$\int_{\mathbb{R}^n} \varphi(x, \bar{x}, \sigma) dx = 1.$$  \hspace{1cm} (33)

3. Requiring in definition A.1 that $\sigma$ is a asymmetric and positive-definite matrix guarantees the existance of the inverse matrix $\sigma^{-1}$ which is also symmetric and positive-definite. This requirement is necessary and sufficient for the existance of the integral (33).

Proposition A.3

1. For the two lowest moments of the $n$-dimensional Gaussian function, i.e., the mean value $E(\varphi)$ and the variance matrix $\text{var}(\varphi)$, one obtains

$$E(\varphi) := \int_{\mathbb{R}^n} x \varphi(x, \bar{x}, \sigma) dx = \bar{x},$$  \hspace{1cm} (34)

$$\text{var}(\varphi) := \int_{\mathbb{R}^n} (x - \bar{x}) \otimes (x - \bar{x}) \varphi(x, \bar{x}, \sigma) dx = \sigma,$$  \hspace{1cm} (35)

where $\otimes$ denotes the tensor product between two vectors.
2. The Fourier transformation of the $n$-dimensional Gaussian integral leads to

$$F^\pm \phi(\cdot, x, \sigma) = \exp(\frac{1}{2} \mathbf{k} \cdot \mathbf{\sigma} \cdot \mathbf{k}) (\det \sigma)^{-1/2} \phi(\cdot, \mathbf{k}, \sigma^{-1})$$

with

$$\mathbf{k} = \mp i \sigma^{-1} \cdot \mathbf{x},$$

where $F^\pm \phi$ denotes the Fourier (inverse Fourier) transformation.

Proof:

The proof of relations (34) to (35) is a generalization of the well-known one-dimensional case [20]. In order to determine the Fourier transformation of $\phi$, one has to evaluate the integral

$$(F^\pm \phi(\cdot, \mathbf{x}, \sigma))(\mathbf{k})$$

$$= (2\pi)^{-n}(\det \sigma)^{-1/2} \int_{\mathbb{R}^n} \exp\left(-\frac{1}{2}(x - x) \cdot \sigma^{-1} \cdot (x - x)\right) \exp \pm i \mathbf{k} \cdot \mathbf{x} \, dx$$

$$= (2\pi)^{-n}(\det \sigma)^{-1/2} \exp \pm i \mathbf{k} \cdot \mathbf{x} \int_{\mathbb{R}^n} \exp\left(-\frac{1}{2}x \cdot \sigma^{-1} \cdot x\right) \exp i \mathbf{k} \cdot \mathbf{x} \, dx$$

$$= (2\pi)^{-n/2} \exp \pm i \mathbf{k} \cdot \mathbf{x} \exp\left(-\frac{1}{2} \mathbf{k} \cdot \mathbf{\sigma} \cdot \mathbf{k}\right),$$

where the relation

$$\int_{\mathbb{R}^n} \exp\left[-\frac{1}{2}(x - x) \cdot \sigma^{-1} \cdot (x - x) - a \cdot (x - x)\right] \, dx$$

$$= (2\pi)^n(\det \sigma)^{1/2} \exp\left[\frac{1}{2} a \cdot \mathbf{a}\right], \quad a \in \mathbb{R}^n$$

was used [20]. With the help of the identity

$$\frac{1}{2} y \cdot A \cdot y \pm ic \cdot y = \frac{1}{2}(y - \bar{y}) \cdot A \cdot (y - \bar{y}) - \frac{1}{2} \bar{y} \cdot A \cdot \bar{y}$$

$$\bar{y} := \mp i A^{-1} \cdot c, \quad y, c \in \mathbb{R}^n, \quad A \in M_n(\mathbb{R}),$$

one obtains

$$(F^\pm \phi(\cdot, \mathbf{x}, \sigma))(\mathbf{k})$$

$$= (2\pi)^{-n/2} \exp\left(\frac{1}{2} \mathbf{k} \cdot \mathbf{\sigma} \cdot \mathbf{k}\right) \exp\left(-\frac{1}{2} \mathbf{k} - \mathbf{k}\right) \cdot \mathbf{\sigma}(\mathbf{k} - \mathbf{k})$$

$$= \exp\left(\frac{1}{2} \mathbf{k} \cdot \mathbf{\sigma} \cdot \mathbf{k}\right) (\det \sigma)^{-1/2} \phi(\mathbf{k}, \mathbf{k}, \sigma^{-1})$$

with

$$\mathbf{k} = \mp i \sigma^{-1} \cdot \mathbf{x}.$$
References


Paper received: 1994-3-24
Paper accepted: 1994-5-6

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