Modelling of anthropogenic pollutant diffusion in the atmosphere and applications to civil protection monitoring

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Abstract

A basic feature of fluid mechanics concerns the frictionless phase-space dynamics of particles in an incompressible fluid. The issue, besides its theoretical interest in turbulence theory, is important in many applications, such as the pollutant dynamics in the atmosphere, a problem relevant for civil protection monitoring of air quality. Actually, both the numerical simulation of the ABL (atmospheric boundary layer) portion of the atmosphere and that of pollutant dynamics may generally require the correct definition of the Lagrangian dynamics which characterizes arbitrary fluid elements of incompressible thermofluids. We claim that particularly important for applications would be to consider these trajectories as phase-space trajectories. This involves, however, the unfolding of a fundamental theoretical problem up to now substantially unsolved: namely the determination of the exact frictionless dynamics of tracer particles in an incompressible fluid, treated either as a deterministic or a turbulent (i.e., stochastic) continuum. In this paper we intend to formulate the necessary theoretical framework to construct such a type of description. This is based on a phase-space inverse kinetic theory (IKT) approach recently developed for incompressible fluids (Ellero et al., 2004-2008). Our claim is that the conditional frictionless dynamics of a tracer particles - which corresponds to a prescribed velocity probability density and an arbitrary choice of the relevant fluid fields - can be exactly specified.

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I. INTRODUCTION

This work (together with Refs. [1]) is a part of a research project related to the theoretical description of pollutant dynamics in the atmosphere, a subject relevant for civil protection monitoring of air quality in the atmosphere. Here, we refer in particular to the so-called ABL (atmospheric boundary layer) portion of the atmosphere where the earth surface (land or water) has a direct influence and most of pollution releases occur. In fact, the ability to predict the dynamics of anthropogenic pollutants, especially in order to estimate their concentration at ground level, is a prerequisite for environmental investigations. A critical issue is therefore the identification of mathematical models, able to give reliable predictions for pollutants concentrations in the presence of complex terrain and for prescribed weather profiles. This involves the ability to simulate pollutant dynamics in a variety of different physical conditions. In fact in the ABL, sufficiently close to the ground, the atmosphere is mainly characterized by a turbulent flow arising from the wind shear produced by friction with the ground surface. Instead, at the top of the ABL, in the free atmosphere, the wind speed is approximately geostrophic and therefore possibly laminar. The stronger the wind, the more intense is the generated turbulence arising close to the ground, whose properties may be very different, depending on the vertical temperature gradient of the atmosphere. Since turbulence reinforces mixing it tends to homogenize the fluid much more quickly than would a laminar flow, thus preventing local accumulation of pollutants. In addition meteorological parameters (of the atmosphere) are strongly affected by the earth’s surface through dynamical processes (friction of the air over the surface and through thermal processes heating or cooling of the air in contact with the ground). Until recently, fully reliable mathematical methods of this type, able to take into account the full complex phenomenology of the atmosphere and simulate the dynamics of particle or gaseous pollutants in the atmosphere, have been missing. For this reason in the past, most of predictions for pollutant transport in the atmosphere have been based on wind-tunnel experiments. Purpose of the presentation is an overview of the mathematical models currently available and a brief analysis of new theoretical developments in the field. In particular, here we intend to refer to the statistical approach developed by Marco Tessarotto et al. [1] based on the IKT (see also Ellero et al., 2000-2008, [2, 3, 4, 5, 6, 26]). In the sequel, we shall concentrate on those issues that we consider mostly relevant for the present investigation. We intend to show that the IKT
approach is a useful theoretical framework that can be used to simulate the dynamics of pollutants in prescribed fluid flows, taking into account, besides the velocity and pressure fields also the temperature of the same fluid. The mathematical approach appears therefore susceptible of actual applications for simulations of pollutants dynamics in the atmosphere, such as those relevant to civil protection monitoring.

II. THE PRESENT STATE OF RESEARCH

The subject of the investigation (pollutant dynamics) involves some of the most disputed and still open issues in fluid dynamics. The motion of particles in a fluid as they are pushed along erratic trajectories by fluctuations of the fluid fields is fundamental to transport and mixing in turbulence. It is essential, for example, in combustion processes [7], in the industrial production of nanoparticles [8] as well as in atmospheric transport, cloud formation and air-quality monitoring of the atmosphere [9, 10]. The Lagrangian approach - denoted as Lagrangian turbulence (LT) - has been fruitful in advancing of the understanding of the anomalous statistical properties of turbulent flows [11]. In particular, the dynamics of particle trajectories has been used successfully to describe mixing and transport in turbulence [7, 12]. Nevertheless, issues of fundamental importance remain unresolved. As it is well known, the description of fluids can be performed choosing either Eulerian or Lagrangian viewpoints. The two approaches are equivalent and, if fluid dynamics were fully understood, one should be able to translate Eulerian properties into Lagrangian ones and viceversa. We are still quite far from this goal.

In the past the treatment of Lagrangian dynamics in turbulence was based on stochastic models of various nature, pioneered by the meteorologist L. F. Richardson [13]. These models, which are based on tools borrowed from the study of random dynamical systems, typically rely - however - on experimental verification rather than on first principles. A first example is provided by refined stochastic models - based in non-extensive statistical mechanics [14, 15] - which try to reproduce the observed intermittency of turbulence [16, 17]. Another approach is based on Brownian-motion-type models, which involve stochastic particle equations of motion and an associated Fokker-Planck equation (see, for example, Subramanian et al.,2004 [18]). In such models the diffusion tensor in the Fokker-Planck equation may depend on the local velocity shear rate, implying a possible violation of the
classical (equilibrium) fluctuation-dissipation theorem [19]. A further class of models has been based on kinetic theory, enabling us to obtain the Fokker-Planck equation for the motion of Brownian particles in rarefied nonuniform gases. In particular, by expanding in term of the mass-ratio (of the light-gas molecular mass to the Brownian-particle mass) the Boltzmann collision operator, the light-gas distribution function was approximated by the first two terms in the Chapman-Enskog expansion. As a result, it was found to obey a Fokker-Planck equation with a diffusion tensor independent of the light-gas velocity gradients [20, 21].

However, in most cases there remains a lack of experimental data to verify the reliability of such models. Verification can be based, in particular, on the measurement of fluid particle trajectories, obtained by seeding a turbulent flow with a small number of tracer particles and following their motions with an imaging system. On the other hand, the accurate evaluation of the Lagrangian velocity in laboratory turbulence experiments requires measurements of positions of tracer particle by using a suitable tracking system able to resolve very short time (and spatial) scales. In practice this can be a very challenging task since particle motions must be measured on very short time scales of the order of the Kolmogorov time,

$$\tau = (\nu/\varepsilon)^{1/2}$$  \hspace{1cm} (1)

where $\nu$ is the kinematic viscosity and $\varepsilon$ the turbulent energy dissipation. Similarly, to get the Lagrangian acceleration one should have experimental access to time scales again comparable or even smaller than the Kolmogorov time scale of the flow. Another important physical observable is the pressure (and the related pressure gradient), which is typically hard to measure experimentally. Despite these difficulties, growing interest in studying Lagrangian turbulence is motivated by the recent advances in laboratory and numerical experiments [22, 23, 24]). In particular, the role of numerical simulations represents a new challenge, since they are expected to represent alternative tools to laboratory experiments.

As for the theory itself, rigorous results have been scanty, probably because of the subject complexity. In particular, an open issue is the very definition of the dynamics of tracer particles which may injected in the fluid with arbitrary initial velocities. These velocities in practice may be generally very different from the local fluid velocity. In contrast, in customary treatments the dynamics of tracer particles is identified with that of the fluid particles, which is determined uniquely by the Navier-Stokes equations. As a consequence, the dynamics
(i.e., in particular the acceleration) of tracer particles in incompressible thermofluids might be very different from that of the fluid elements. This problem is not only a challenging theoretical issue, but is obviously of primary importance for its implications in computational and environmental fluid dynamics.

In this connection, however, recently there has been an important breakthrough, represented by the discovery of the so-called inverse kinetic theory (IKT) approach for incompressible fluids [2, 3, 4, 5, 6]. In accompanying papers [1, 25] the same approach has been extended to the treatment of incompressible thermofluids.

In this paper we claim that the IKT of Ref. [1] permits us to determine uniquely the (frictionless) dynamics of tracer particles.

In fact, a key feature of the this type of approach is that it affords a straightforward connection between Eulerian and Lagrangian fluid descriptions. This is achieved by identifying the relevant fluid fields, which are assumed to be defined in a suitable domain \( \Omega \subseteq \mathbb{R}^3 \) (fluid domain), with appropriate moments of a suitably-defined kinetic distribution function density \( f(x,t) \) [with \( x = (r, v) \in \Gamma, x \) and \( \Gamma \) denoting a suitable state-vector and an appropriate phase-space] which is assumed to advance in time by means of Vlasov-type kinetic equation. In such a case, the time-evolution of the kinetic distribution function is determined by a kinetic equation which, written in the Eulerian form, reads

\[
Lf(x, t) = 0.
\]  

(2)

Here \( L \) is the streaming operator \( Lf \equiv \frac{\partial}{\partial t} f + \frac{\partial}{\partial x} \cdot \{X(x, t)f\} \) and \( X(x, t) \equiv \{v, F(x, t)\} \) a suitably smooth vector field, while \( v \) and \( F(x, t) \) denote respectively appropriate velocity and acceleration fields. As a main consequence the approach can in principle be used to determine in a rigorous way the Lagrangian formulation for arbitrary complex fluids. Although the choice of the phase space \( \Gamma \) is in principle arbitrary, in the case of incompressible isothermal fluids, it is found [3] that the phase-space \( \Gamma \) can always be reduced to the direct-product space \( \Gamma = \Omega \times V \) (restricted phase-space), where \( \Omega, V \subseteq \mathbb{R}^3, \Omega \) is an open set denoted as configuration space of the fluid (fluid domain) and \( V \) is the velocity space. This type of approach (based on a restricted phase-space IKT formulation) will be adopted also in the sequel. The main motivation [of this work] is that some of the general understanding recently achieved in simple flows by means of the IKT approach could also give a significant contribution to a wider range of problems. In the sequel, we will
concentrate on the issue of a consistent Lagrangian formulation for fluid dynamics based on a phase-space (IKT) description of incompressible fluids, whereby its pressure, velocity (and possibly also thermal) fluctuations are consistently taken into account in the phase-space dynamics of suitable phase-space inertial particles, i.e., particles whose dynamics is determined by the phase-space Lagrangian characteristics. The motion of these particles, as they are pushed along erratic trajectories by fluctuations of the fluid-field gradients (in particular, characterizing the fluid pressure and temperature), is fundamental to transport and mixing processes in fluids. It is well known that the interaction between (deterministic and/or turbulent) fluctuations of the fluid fields and these particles still escapes a consistent theoretical description. Being a subject of major importance for many environmental, geophysical and industrial applications, the issue deserves a careful investigation. A key aspect of fluid dynamics is the correct definition of the (phase-space) Lagrangian dynamics which characterizes incompressible fluids. The customary approach to the Lagrangian formulation is based typically on a configuration-space description, i.e., on the introduction of the configuration-space Lagrangian characteristics \( r(t) \), spanning the fluid domain \( \Omega \). Here \( r(t) \) denotes the solution of the initial-value problem:

\[
\begin{align*}
\frac{dr}{dt} &= V(r, t), \\
r(t_o) &= r_o,
\end{align*}
\]

with \( r_o \) an arbitrary vector belonging to the closure \( \overline{\Omega} \) of \( \Omega \) and \( V(r, t) \) being the velocity fluid field, to be assumed continuous in \( \overline{\Omega} \) and suitably smooth in \( \Omega \). In a previous paper [1], IKT has been proven to advance in time self-consistently the fluid fields, i.e., in such a way that they satisfy identically the requires set of fluid equations. For isothermal fluids, this conclusion is consistent with the results indicated elsewhere by Tessarotto et al. [4]. In particular, basic feature of the IKT approach is to permit to advance in time the fluid fields only by means of suitable evolution equations, without requiring the (numerical) solution of the Poisson equation for the fluid pressure. The purpose of this paper is to point out that, based the same approach [1] for incompressible thermodfluids, the dynamics of tracer particles, of finite mass \( m_T \), which are injected in the fluid with arbitrary velocity, can be rigorously established.
III. THE EXACT FRICTIONLESS CONDITIONAL DYNAMICS OF TRACER PARTICLES

In this Section we intend to show that the equations of motion for a tracer particle in an incompressible fluid can be uniquely specified, once the velocity probability density are prescribed (conditional dynamics). For definiteness in the sequel we shall consider an incompressible thermofluid, described by the fluid fields \( \{ \rho = \rho_o > 0, V, p \geq 0, T > 0 \} \), denoting respectively the (constant) mass density, fluid velocity, pressure and temperature describing the fluid. The fluid fields are assumed to be suitably smooth, classical solutions of the incompressible Navier-Stokes-Fourier equations (INSFE problem, [1]), all defined in a bounded connected set (fluid domain) \( \Omega \subseteq \mathbb{R}^3 \) (with \( \overline{\Omega} \) denoting its closure set where the mass density \( \rho \) is strictly positive):

\[
\nabla \cdot V = 0,
\]

\[
\frac{D}{Dt} V = - \frac{1}{\rho_o} [\nabla p - f] + \nu \nabla^2 V,
\]

\[
\frac{D}{Dt} T = \chi \nabla^2 T + \frac{\nu}{2c_p} \left( \frac{\partial V_i}{\partial x_k} + \frac{\partial V_k}{\partial x_i} \right)^2 + \frac{1}{\rho_o c_p} J \equiv K.
\]

In standard notation, \( \frac{D}{Dt} V \) denotes the fluid acceleration, with \( \frac{D}{Dt} = \frac{\partial}{\partial t} + V \cdot \nabla \) the convective derivative, \( J \) is the quantity of heat generated by external sources per unit volume and unit time and finally \( f \) is the force density for which the Boussinesq approximation is invoked. Hence, \( f \) is taken on the form \( f = \rho_o g (1 - k_\rho T) + f_1 \), where the first term represents the (temperature-dependent) gravitational force density and the second one (\( f_1 \)) the action of a possible non-gravitational externally-produced force density. As a consequence, in such a case the force density \( f \) reads \( f = \rho_o g (1 - k_\rho T) + f_1 \), where the first term represents the (temperature-dependent) gravitational force density, while the second one (\( f_1 \)) the action of a possible non-gravitational externally-produced force. Hence \( f \) can be written also as \( f = - \nabla \phi + f_R \), where \( \phi = \rho_o g z \) and \( f_R = - \rho_o g k_\rho T + f_1 \) denote respectively the gravitational potential (hydrostatic pressure) and the non-potential force density. Finally, \( \nu, \chi, c_p \) and \( k_\rho \) are all real positive constants which denote, respectively, the kinematic viscosity, the thermometric conductivity, the specific heat at constant pressure, and the density thermal-dilatation coefficient. A remarkable aspect of fluid dynamics is related to the construction of IKT’s for hydrodynamic equations in which the fluid fields are identified with suitable moments of an appropriate kinetic probability distribution. This is achieved introducing a
phase-space classical dynamical system (CDS)

\[ x_o \rightarrow x(t) = T_{t,t_o} x_o, \]  

which uniquely advances in time the fluid fields by means of an appropriate evolution operator \( T_{t,t_o} \). The CDS is assumed to be generated by the initial-value problem associate to the Lagrangian equations

\[ \begin{align*}
\frac{d}{dt} r(t) &= v(t), \\
\frac{d}{dt} v(t) &= F(r(t), t; f), \\
r(t_o) &= r_o, \\
v(t_o) &= v_o,
\end{align*} \]  

where \( x = (r, v) \in \Gamma \) and respectively \( r \) and \( v \) denote an appropriate state-vector and the corresponding configuration and velocity vectors. Moreover \( X(x, t) \equiv \{v, F(x, t; f)\} \) is a suitably smooth vector fields, with \( F(x, t; f) \) representing an acceleration field. It is assumed that generally \( F(x, t; f) \) can depend functionally on \( f \equiv f(x, t) \), to be identified with a suitable probability density function (pdf). In particular, let us require that \( x \) spans the phase-space \( \Gamma = \Omega \times V \), where \( V = \mathbb{R}^3 \) denotes the velocity space. Therefore, introducing the corresponding velocity pdf \( f(x, t) \), defined so that

\[ \int_V d^3v f(x, t) = 1, \]  

in \( \Gamma \) it fulfills necessarily the integral Liouville equation

\[ J(t) f(x(t), t) = f(x_o, t_o). \]  

Here, \( x(t) \) denotes the Lagrangian path determined by the CDS, which is assumed to be a diffeomorphism at least of class \( C^2(\Gamma \times I \times I) \), with \( I \subset \mathbb{R} \) denoting an appropriate finite time interval, and \( J(t) = \left| \frac{\partial x(t)}{\partial x_o} \right| \) is corresponding Jacobian. Then, if the initial pdf \( f(x_o, t_o) \) is suitably smooth, it follows that the time-evolved pdf \( f(x, t) \) satisfies necessarily the differential Liouville equation

\[ L f(x, t) = 0, \]  

where \( L \) denotes the Liouville streaming operator. This equation (inverse kinetic equation), which may be interpreted as a Vlasov-type kinetic equation, can in principle be defined in such a way to satisfy appropriate constraint equations. In particular, thanks to the
arbitrariness of the dynamical systems (7), the velocity moments of \( f(x,t) \) can be identified so that suitable velocity moments of \( f \) coincide with the relevant fluid fields which characterize an incompressible thermofluid. In particular, introducing the kinetic pressure \( p_1 \), defined so that

\[
p_1 = p_0(t) + p - \phi + \rho_o T/m,
\]

we can identify \( m \) with the average molecular mass of the classical molecules forming the fluid and the ratio \( \rho_o/m \equiv n_o \) with the fluid number density \( n_o \) of the fluid. In such a case, imposing the constraints \( \mathbf{V} \cdot p_1 = \int \rho_o \mathbf{v} G(x,t) f(x,t) \), respectively for \( G(x,t) = \mathbf{v} \), \( \rho_o (\mathbf{v} - \mathbf{V})^2/3 \), and subject to the requirement of strict positivity and regularity for \( f(x,t) \), the correct form of the acceleration field \( \mathbf{F} \equiv \mathbf{F}(x,t;f) \) can be proven to be [1]:

\[
\mathbf{F}(x,t;f) = \mathbf{F}_0 + \mathbf{F}_1,
\]

where \( \mathbf{F}_0, \mathbf{F}_1 \) read respectively

\[
\mathbf{F}_0(x,t;f) = \frac{1}{\rho_o} \left[ \nabla \cdot \mathbf{Q} - \nabla p_1 + \mathbf{f}_R \right] + \mathbf{u} \cdot \nabla \mathbf{V} + \nu \nabla^2 \mathbf{V},
\]

\[
\mathbf{F}_1(x,t;f) = \frac{1}{2} \mathbf{u} \left\{ \frac{1}{p_1} A + \frac{1}{p_1} \mathbf{Q} - \frac{1}{p_1} \left[ \nabla \cdot \mathbf{Q} \right] \cdot \mathbf{Q} \right\} + \frac{\nu^2}{2} \frac{\mathbf{v}_{th}^2}{p_1} \nabla \cdot \mathbf{Q} \left\{ \frac{u^2}{\rho_o \mathbf{v}_{th}^2} - \frac{3}{2} \right\},
\]

and

\[
A - \frac{\partial}{\partial t} (p_0 + p) - \mathbf{V} \cdot \left[ \frac{D}{Dt} \mathbf{V} - \frac{1}{\rho_o} \mathbf{f}_R - \nu \nabla^2 \mathbf{V} \right] + \frac{\rho_o K}{m},
\]

\[
K = \chi \nabla^2 T + \frac{\nu}{2c_p} \left( \frac{\partial V_i}{\partial x_k} + \frac{\partial V_k}{\partial x_i} \right)^2 + \frac{1}{\rho_o c_p} J.
\]

Here the notation is given in accordance with Ref. [1]. Thus, \( p_0(t) \) (to be denoted as pseudo-pressure [4]) is a suitably-defined, strictly positive and smooth real function, to be determined to assure the validity of an H-theorem (and hence the strict positivity of \( f(x,t) \), \( \mathbf{Q} \) and \( \Pi \) denote the additional velocity moments \( \mathbf{Q} = \rho_o \int d^3 v u u^2 f \) and \( \Pi = \rho_o \int d^3 v \mathbf{u} \mathbf{u} f \)).

The following consequences are implied by the previous Lagrangian equations (8) [together with the definitions (13)-(12)]:

1. the Lagrangian equations (8) can be interpreted either as deterministic or stochastic, depending whether the fluid fields themselves are treated as such (see also Ref. [26]);
2. $F(x, t; f)$ can be interpreted as the "conditional" Lagrangian acceleration, which depends functionally on the form of the pdf $f(x,t)$. In particular, in the case of a turbulent fluid also the pdf must be considered as stochastic [26];

3. it is possible to prove that the functional form of the vector field $F(x, t; f)$ can be uniquely specified once $f(x,t)$ is prescribed;

4. the form of $f(x,t)$ is determined uniquely by its initial condition $f(x_o, t_o)$ [see Eq.(11)] and by the time-evolution operator $T_{t,t_o}$;

5. in turn, $T_{t,t_o}$ is defined uniquely by the CDC (7) $f(x,t)$;

6. a particular solution of Eq.(11) is delivered by the Maxwellian pdf

$$f_M(x, t) = \frac{1}{\pi^2 v_{th,p}^3} \exp \left\{-\frac{u^2}{v_{th,p}^2}\right\},$$

where $u = v - V(r, t)$ and $v_{th,p} = \sqrt{2p_1(r, t)/\rho}$ are respectively the relative and the thermal velocities.

7. the case of an isothermal fluid is recovered by imposing that there results identically $T(r, t) = \text{const.}$ and $K \equiv 0$ [see the r.h.s. of Eq.(8)].

We conclude that, the Lagrangian equations [8], when letting $m = m_T$, define the equations of motion for a tracer particle with initial conditions $\{r(t_o), v(t_o)\} = (r_o, v_o)$ and subject to the conditional acceleration $F(x, t; f)$.

IV. CONCLUSION AND OUTLOOK

In this Note we have proven that the exact dynamics of tracer particles injected in incompressible thermofluids can be rigorously established. The result appears relevant not only from the theoretical viewpoint but also for its applications and in particular for the description and monitoring of pollutant dynamics in the atmosphere.

We stress that only weak restrictions have been assumed on the form of the pdf, affecting the form of the conditional acceleration $F(x, t; f)$. In addition, the theory applies in principle to arbitrary fluid fields which are strong solutions of the INSFE problem. Therefore, this permits in principle also the proper treatment of turbulent, i.e., stochastic fields. As a
consequence, the formulation here presented is susceptible of applications in turbulence theory.

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**Notice**

§ contributed paper at RGD26 (Kyoto, Japan, July 2008).
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