The Generalized Kinetic Modelling of a Multicomponent "Real-Life" Fluid by Means of a Single Distribution Function

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Abstract—This work proposes a fully continuum stochastic model of a multicomponent fluid. It is shown that the way to this model leads to a generalized-kinetics (GK) theory. Subsequently, the model is developed as a corresponding extension of this theory. The obtained model presents the overall generalized distribution function. It is described with a nonlinear nonlocal (or "mean-field") system of two scalar equations, no matter how many components are in the fluid, and a special prescription. The system comprises

(i) the generalized kinetic equation for the conditional distribution function conditioned with the values of the particle-property stochastic process, and
(ii) the McKean-Kolmogorov forward equation for the probability density of this process.

The aforementioned prescription determines the number of the fluid components as the number of the modes of this density. The work also includes a theorem that provides an estimation from below for this number in the generic stationary case of the corresponding multidimensional Kolmogorov equation and points out how the modes manifest themselves in the drift and diffusion functions (more specifically, in the Fichera drift function). The discussion on the model and a few directions for future research concludes the work. © 2003 Elsevier Ltd. All rights reserved.

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1. INTRODUCTION

Much experimental evidence demonstrates that biological phenomena are radically more complex than those usually studied in physics and chemistry by statistical mechanics. The key issues on that are discussed in [1]. The main phenomena and other related features are listed below.

(a) Biological fluids, the sets of discrete entities in what follows, called particles and interacting with the surrounding of the fluid and with each other, usually comprise hundreds or
thousands of different fluid components, i.e., populations of identical bioparticles. The components are not always clearly defined. The number of the components generally varies in time.

(b) Bioparticles (cells, molecules, proteins, ions, etc.) are disparate: they strongly differ in the geometrical, mechanical, and biophysical properties. Bioparticles often have intricate internal structures. This also leads to unprecedented diversity in the interparticle interactions involving those of complicated types, for instance, the inherently mean-field interaction.

(c) The properties of the bioparticles and the contents of the components are generally of a noticeable irregularity which varies in both time and physical space. In other words, biosystems can generally be regarded as spatially distributed stochastic structures (cf. [2]). These structures play a key role in the advanced, deductive vision of biology [3].

(d) Along with this, the fluid components can sometimes include as low as a few particles each. If so, they cannot be treated by means of averaging over a statistically large number of particles, the procedure which is the core of statistical mechanics (e.g., [4]). Subsequently, the vision of fluctuations which is common in physics and chemistry and assigns fluctuations to stem from interactions of a large number of particles needs to be revised.

(e) The bioparticle populations are located in bounded, often, mesoscale (say, a-few-tens-of-micrometer-size) (cf. [5]) domains where the finite-size effects are generally of importance and, therefore, cannot be neglected. As a result, the macroscopically-large (infinite-in-the-limit)-domain assumption involved in the averaging in Point (d), i.e., the so-called thermodynamic limit (TDL) (e.g., [4,6,7,8, (4.6) p. 111]) is, in general, inapplicable to biological problems.

Dealing with problems related to Points (b) and (c) can be based on the generalized-kinetics (GK) theory (e.g., see [9-11] and the literature therein). Here the diversity and randomness of the particle properties is flexibly accounted by the generalized distribution functions and the corresponding generalized kinetic equations (e.g., [11, Section 2]). However, methods of kinetic theory can be applied only in the dilute-fluid approximation, while various biological fluids can be modeled only if the above Items (b) and (c) are properly dealt with. A possible way to overcome the difficulties in Points (d) and (e) is suggested by a nonequilibrium nonlinear stochastic hydrodynamics (NNSHD) [12,13]. This treatment is comparable with the stochastic kinetic equations (e.g., the stochastic Boltzmann equation also known as the Boltzmann-Langevin equation), but noticeably simpler (and even somewhat more general). The NNSHD development can pertain to the research trends (e.g., [9-11,14-16]) in the mechanical treatments which are free from certain limitations of statistical mechanics.

The purpose of the present work is to contribute to solutions of the problem in Point (a) by means of the corresponding extension of the above GK approach. More specifically, the developed extension is to be a fully continuum paradigm of multicomponent fluids including those of large numbers of the components. Section 2 presents a continuum generalization of the multicomponent-fluid picture that leads to the above generalized distribution functions for the components. This vision is summarized briefly in Section 3. Section 4 extends the preceding considerations with the notion of the overall generalized distribution function, a single function describing the whole set of the fluid components. In so doing, the components are interpreted in terms of the modes of certain probability density. Subsequently, the property of a fluid to be multicomponent corresponds to the property of this density to be multimodal. Section 5 unifies the treatments in Sections 3 and 4. Here the probability density is presented as the probability density for the properties of the fluid particles. It, together with the conditional distribution function (conditioned with the particle-property values) and the number of the modes, composes the overall generalized distribution function. The model to determine it is proposed in Section 6 in the form of a system of the following two coupled nonlinear scalar equations. One of them is
the generalized kinetic equation for the conditional distribution function, whereas the other one is the McKean-Kolmogorov forward equation for the particle-property probability density.

This system includes a profound nonlocal memory effect. Section 7 includes the theorem which provides an estimation from below for the mode number in the generic stationary case of the corresponding multidimensional Kolmogorov equation and points out how the modes manifest themselves in the drift and diffusion functions. Section 8 summarizes the proposed modelling and suggests a few directions for future research.

The work follows the conventions below.

Equation (X.Y) denotes the Yth equation in Section X. Remark X.Y or Example X.Y denotes the Yth remark or the Yth example in Section X. For the sake of space, the conditions allowing us to carry out most of common operations in the course of consideration are assumed to hold and not formulated in the text. In particular, all the integrals dependent on parameters are regarded to be sufficiently smooth functions of respective parameters. It is also assumed that all the multifold integrals can be evaluated in any order of the integration, and all the corresponding intermediate integrals are sufficiently regular (e.g., smooth) functions of their variables.

For reader’s convenience, all the function symbols are typed in bold. In so doing, the symbol is the same as the plain-typed symbol for the variable described by the bold-typed function. For example, if a variable is denoted with x (plain “z”), then the function for it is denoted with x (bold “z”), no matter whether the symbols are typed in italics or not. Moreover, all the functions unavailable (until now) in statistical mechanics are marked with the subscript “*” (e.g., q*).

2. A MULTICOMPONENT FLUID: FROM COMMON TO GENERALIZED DISTRIBUTION FUNCTIONS

This work deals with a fluid which occupies a domain (i.e., open connected set) \( \Omega(t) \subseteq \mathbb{R}^3 \) with piecewise smooth boundary \( \partial \Omega(t) \) where \( t \) is the time, \( t \in \mathbb{R}, \mathbb{R} = (-\infty, \infty). \) In so doing, the focus is on the general case when the fluid is multicomponent.

2.1. Common Kinetic Modelling of a Multicomponent Fluid

A one-component fluid is a fluid composed by identical particles, i.e., the particles with the same properties. A multicomponent fluid is a fluid which consists of one or more one-component fluids called the components of the multicomponent fluid. The latter is called the \( M_0 \)-component fluid, \( M_0 \geq 1 \), when it consists of exactly \( M_0 \) components. If \( M_0 \geq 2 \), then all the components are pairwise different. Note that, as follows from Point (a) in Section 1, for biological fluids,

\[
\text{number } M_0 \text{ can be on the order of hundreds or thousands.} \quad (2.1)
\]

Remark 2.1. On one hand, the assumption that the fluid particles are identical is a strong idealization. In the real-life fluids, particles are normally far from being identical. On the other hand, the aforementioned assumption is a prerequisite for introduction of the so-called reduced distribution functions (e.g., [8, Section 1.6.3]; see also the text below (2.5)), one of the cornerstones of statistical mechanics. This science, in its attempts to pull the above assumption in the real-life fluids, suggested an introduction of the fluid components, i.e., the groups of the particles where the particles in different groups are different, but the particles in the same group are not allowed to be nonidentical. In so doing, the number of the components is fixed. In other words, statistical-mechanics models for any fluid are built up according to a clear and stiff scheme.

However, it still remains unclear how the resulting, imaginary world of fluids corresponds to the real-life problems. What if the particles in a component tend to be different? What if properties of the particle are varying in time and space assigning it to different components within different intervals of motion? What if the component number varies in time and in a random manner or is merely unknown in advance? What if a mixture of fluids is so complex that
even a formulation of the components, not to mention analysis of the mixture, is a challenging problem? To our knowledge, in the statistical-mechanics literature, there are no consistent recipes on how to tie down the actual diversity of particles of fluids to the frames of the above different-components/identical-particles scheme.

In spite of the numerous unsolved problems in Remark 2.1, the present analysis follows the traditional vision to the very end of Section 2.3. In common kinetic theory (e.g., [8, Section 3.2.2; 17,18]), an $M_o$-component fluid, $M_o \geq 1$, is described (e.g., [8, Section 3.2.2]) with $M_o$ distribution functions $f_1, \ldots, f_{M_o}$ of variable $(t, X, V)$ where vectors $X \in \Omega(t), V \in \mathbb{R}^3$ represent values of the particle-position and particle-velocity vectors $x$ and $v$, respectively. These functions are usually of the properties below:

\begin{align*}
  f_i(t, X, V) &\geq 0, \quad M_o \geq 1, \quad i = 1, \ldots, M_o, \quad t \geq t_o, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad (2.2) \\
  \text{function } f_i \text{ is a sufficiently regular with respect to all its variables} \\
  M_o \geq 1, \quad i = 1, \ldots, M_o, \quad (2.3) \\
  N_i(t) &> 0, \quad t \geq t_o, \quad M_o \geq 1, \quad i = 1, \ldots, M_o. \quad (2.4)
\end{align*}

where $t_o \in \mathbb{R}$ is the initial time point.

In statistical mechanics, function $f_i$, $i = 1, 2, \ldots, M_o$ is known as the so-called reduced one-particle distribution function (e.g., [8, Section 1.6.3; 4, p. 38]). It describes the populations of the particles in the $i$ components of the fluid. Note that, if $M_o \geq 2$, functions $f_1, \ldots, f_{M_o}$ are pairwise different, but are in general pairwise functionally dependent. The distribution function $f_o$ for the entire $M_o$-component fluid, i.e., the total distribution function, is determined as follows:

\[ f_o(t, X, V) = \sum_{i=1}^{M_o} f_i(t, X, V), \quad M_o \geq 1, \quad t \geq t_o, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3. \quad (2.6) \]

This is the main distribution function describing the fluid.

**Remark 2.2.** The common model (2.2)-(2.6) suggests that we solve a system of $M_o$ kinetic, integro-differential equations for $M_o$ distributions functions $f_1, \ldots, f_{M_o}$ of seven scalar variables each (e.g., see system (6.1) below). This approach does not seem to be practical in case (2.1), since it then leads to a huge kinetic-equation system of a prohibitive complexity. Thus, case (2.1) requires the modelling alternatives that are more compact.

We will see below that relation (2.6) can serve as a starting point for a more compact and considerably more general vision of multicomponent fluids.

### 2.2. The Component- and Particle-State Vector Variables

The formulations in Section 2.1 presuppose the ability to distinguish the properties of the fluid particles. Assume one can do that with respect to a finite number of these properties, say, $l + m$, $l, m \geq 1$, and each property can be quantified with a real scalar variable. This means that the set of the properties is described with $l + m$-dimensional vector, say,

\[ q = \begin{pmatrix} u \\ z \end{pmatrix}, \quad (2.7) \]

in what follows called the particle-property vector variable. Vector $u = (u_1, \ldots, u_l) \in \mathbb{R}^l$ in (2.7) denotes the particle properties which determine the number of the components of the
fluid. This vector is called the component-state vector variable. In contrast to it, vector \( z = (z_1, \ldots, z_m) \in \mathbb{R}^m \) in (2.7) denotes the particle properties which do not affect the component number determined by vector \( u \). Vector \( z \) is called the particle-state vector variable. The \( j^{\text{th}} \) entry \( u_j \) of vector \( u \) (or the \( j^{\text{th}} \) entry \( q_j \) of vector \( q \)) corresponds to the \( j^{\text{th}} \) property related to the component state, \( j = 1, \ldots, l \), whereas the \( j^{\text{th}} \) entry \( z_j \) of vector \( z \) (or the \((l+j)^{\text{th}} \) entry \( q_{l+j} \) of vector \( q \)) corresponds to the \( j^{\text{th}} \) property related to the particle state, \( j = 1, \ldots, m \).

**EXAMPLE 2.1.** If one considers mobile electrons and holes in a semiconductor, then one can set \( l, m = 1 \), \( u_1 \) is the particle charge, and \( z_1 \) is the particle mass. The values of the charges of the above particles are sharply different: they are of the opposite signs. These values determine two components of the electron-hole fluid. Hence, it is reasonable to present the particle charge with an entry of the component-state vector \( u \). On the contrary, the values of the masses of the above particles usually do not differ from each other very much. They do not determine any additional component of the fluid, thereby explaining why the particle mass can be presented with an entry of the particle-state vector \( z \). This simple example merely illustrates the above paragraph and is not a comprehensive description of semiconductor-related charge-carrier fluids.

**EXAMPLE 2.2.** An important parameter of a particle is its spin \( s \), a scalar quantity associated with the particle quantum-mechanical intrinsic angular momentum. The number \( s \) is such that \( 2s \) is a nonnegative integer. The particles with odd values of \( 2s \) are known as fermions. At equilibrium, they obey the Fermi-Dirac distribution. The particles with even values of \( 2s \) are known as bosons. At equilibrium, they obey the Bose-Einstein distribution. In the limit case when the particle concentration tends to zero, both the FD and BE distributions are reduced to the Maxwell-Boltzmann distribution. Electrons, positrons, protons, neutrons, and quarks are examples of fermions. Photons, pions, gluons, \( \pi \) mesons, \( K \) mesons, the deuteron, and the \( \alpha \)-particle are examples of bosons. The following rules are well known (e.g., [19, p. 251]; see also [20] for the details and applicability conditions). Composite particles of bosons are bosons. Composite particles of an even number of fermions are also bosons. Composite particles of an odd number of fermions are fermions.

Many examples of bosons and fermions can be found in biology. One of them concerns hemoglobin, an iron-containing protein pigment occurring in red blood cells of vertebrates and functioning primarily in the transport of oxygen from the lungs to the tissues of the body. The \( \text{Fe}^{2+} \) and \( \text{Fe}^{3+} \) ions are components of hemoglobin. In so doing [21, Table 1], the \( \text{Fe}^{2+} \) ions act as bosons with \( s = 0 \) or \( s = 2 \), whereas the \( \text{Fe}^{3+} \) ions act as fermions with \( s = 1/2 \) or \( s = 5/2 \).

The above spin picture can be expressed in terms of vector (2.7) in the following way. One sets \( l, m \geq 1 \), \( z_1 = s \), and \( u_1 = (-1)^{2z_1+1} \) is the particle spin type, i.e., \( u_1 = -1 \) for boson and \( u_1 = 1 \) for fermion.

The notion of the component-state vector is new in the GK theory. The notion of the particle-state vector is known in the GK theory as a microscopic [9, p. 315; 11, Section 2] or functional ([10, Section 3]; see also Point (iii) in [10, Section 9]) state. This state pertains [9, p. 2] to single individuals, i.e., the particles of a fluid, and to their interaction. For this reason, in the present work, the microscopic (or functional) state is, termed the particle state. This term also attracts attention to the properties of the fluid particles. The interaction-related aspects (the forms of the corresponding equations) are considered in Sections 6 and 7. The rest of the present section and Section 3 deal with the particle-state vector variable, whereas Section 4 focuses on the component-state vector variable. The unified vision is presented in Section 5.

### 2.3. Common Distribution Functions from the Viewpoint of the Component- and Particle-State Vectors

This section and the next one, as well as Section 3, deal with the reformulation of the modelling in Section 2.1 in terms of the values of vector \( z \) described in Section 2.2.
Remark 2.3. It is important to recognize that vector variables \( u \) and \( z \)

- for a one-component fluid, are described with a single distribution function \( f_l \) and have single values, \( U_1 \) and \( Z_1 \), fixed \( l \)- and \( m \)-vectors;
- for an \( M_o \)-component fluid, \( M_o \geq 2 \), are described with \( M_o \) pairwise different distribution functions \( f_{1}, \ldots, f_{M_o} \), have \( M_o \) values \( U_1, \ldots, U_{M_o} \) and \( Z_1, \ldots, Z_{M_o} \) such that fixed \( l \) - and \( m \)-vectors \( U_i \) and \( Z_i \) correspond to the \( i^{th} \) component with distribution \( f_i \) and

\[
U_i \neq U_j, \quad M_o \geq 2, \quad i, j = 1, \ldots, M_o : i \neq j. \tag{2.8}
\]

From the point of view of the treatment in Section 2.1, the fixed values \( U_1, \ldots, U_{M_o} \) and \( Z_1, \ldots, Z_{M_o}, M_o \geq 1 \), are nothing but a part of the input data: they cannot be derived within this treatment. Other, microscopic approaches, i.e., those which deal with the properties of the very particles of the fluid, must be used.

Also note that, at \( l \geq 2 \) and \( M_o \geq 2 \), pairwise different \( l \)-vectors \( U_1, \ldots, U_{M_o} \) generally differ from each other in any number of the \( l \) entries and are, thus, incomparable with each other. For this reason, the components of the \( M_o \)-component fluid are generally disparate, so the latter can be regarded as an \( M_o \)-component mixture of the disparate fluids.

One of the alternatives in Remark 2.2 may be associated with the generalization of the function set \( f_1, \ldots, f_{M_o} \) of variable \( (t, X, V) \) to a single function, say, \( f \) of variable \( (t, X, V, U, Z) \) which

- as a function of values \( U \) and \( Z \) of vectors \( u \) and \( z \), i.e., value

\[
Q = \begin{pmatrix} U \\ Z \end{pmatrix} \tag{2.9}
\]

of vector (2.7), is defined on the corresponding continuum set, say, domains (i.e., open connected sets) \( Y_*(t) \subseteq \mathbb{R}^l \) and \( Z_*(t) \subseteq \mathbb{R}^m \), respectively, and

- provides the corresponding continuum reading of relation (2.6) which can be started with expressions

\[
f_l(t, X, V) = \int_{\mathbb{R}^m} f_l(t, X, V) \delta_m(Z - Z_i) dZ,
\]

\[
M_o \geq 1, \quad i = 1, \ldots, M_o, \quad t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \tag{2.10}
\]

for functions \( f_1, \ldots, f_{M_o} \), the terms in (2.6), where \( \delta_m \) is the Dirac delta-function in \( \mathbb{R}^m \).

This topic is considered from the next section down to Section 4. Section 4 suggests a continuum generalization of the summation in (2.6).

2.4. The Continuum Generalization of the Approach of Section 2.1

The above generalization can be achieved if one involves the notions of component- and particle-state vectors from Section 2.2 and the issues in Remark 2.3 by means of the two steps below.

Expression (2.10) presumes that the particle-state vector \( z \) is presented with a random variable, say, i.e., \( z = z(\cdot) \) where \( z \) is a function of elementary event \( \xi \in \Sigma, \Sigma \) is the space of elementary events. Indeed, each function \( \delta_m(-Z_i) \) in (2.10) can be interpreted as the \( i^{th} \)-component version of the probability density of the particle-state random variable \( z(\cdot) \). A generalization of these versions is the first step towards a continuum paradigm pointed out below Remark 2.3.

Let function \( \nu_*(t, U, \cdot) \) of variable \( Z \) be defined with the following properties:

- function \( \nu_*(t, U, \cdot) \), \( t \geq t_0, U \in Y_*(t) \), is the conditional probability density conditioned with value \( U \) of variable \( u \) at time \( t \),

\[
\nu_*(t, U, \cdot) \tag{2.11}
\]

- function \( \nu_* \) is sufficiently regular with respect to all its variables.
Now we replace $\delta_m(\cdot - Z_i)$ and $M_0$ in (2.10) with $v_*(t, U_i, \cdot)$ and $M$, respectively. As a result, we obtain

$$f_i(t, X, V) = \int_{\Omega_*(t)} f_i(t, X, V)\nu_*(t, U_i, Z) dZ,$$

(2.13)

$$M \geq 1, \quad i = 1, \ldots, M, \quad t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U_i \in Y_*(t).$$

Passing from probability densities $\delta_m(\cdot - Z_i)$ to $\nu_*(t, U_i, \cdot)$, i.e., the conditional probability density (see (2.11)) conditioned with value $U_i$, generalizes the $i$th-component versions of the particle-state random variable $\tau(\cdot)$ to the corresponding versions of the particle-state stochastic process. We denote this process with $z_*(\cdot, \cdot)$, so $z = z_*(\xi, t)$.

**Remark 2.4.** Probability densities $\delta_m(\cdot - Z_i)$ (see (2.10)) are very special: they describe random variables which are in fact nonrandom. Passing from them to a general probability densities $\nu_*(t, U_i, \cdot)$ (see (2.13)) in many specific problems enables one to revise the set of the fluid components. Indeed, the components corresponding to the values $U_i$ which are not very much different from each other (or different groups of similar components) can be collected in a single unifying component (or in a few unifying components), thereby noticeably reducing the number of the components from $M_0$ to, say $M$, where

$$M \gg M_0.$$  

(2.14)

(A deterministic and simple example of this procedure is commonly used in connection with the electron-hole fluids in semiconductor theory of crystalline silicon (see also, Example 2.1). Here the electrons in the six valleys of the conduction band are regarded as one component of the fluid, whereas the holes in the three different subbands of the valence band are regarded as another component of the fluid.)

These issues also explain the aforementioned passing from $M_0$ to $M$. However, in general, the above revision of the fluid components alone cannot provide very low values of the resulting number $M$ of the fluid components. This number can still be high. For instance, in case (2.1), for biological fluids, one expects that

$$\text{number } M \text{ can be on the order of tens or hundreds.}$$  

(2.15)

In other words, feature (2.14) is the contribution of $\nu_*(t, U_i, \cdot)$ to resolving the problem in Remark 2.2 rather than a solution of the problem.

The second step is analogous to the first one but concerns distribution functions $f_1, \ldots, f_M$ in (2.13) (rather than probability densities $\delta_m(\cdot - Z_i)$ in (2.10)). Let function $f_*$ of variable $(t, X, V, U, Z)$ be defined with the following properties:

$$f_*(t, X, V, U, Z) \geq 0, \quad t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U \in Y_*(t), \quad Z \in Z_*(t), \quad (2.16)$$

function $f_*$ is sufficiently regular with respect to all its variables,  

$$0 < N_*(t, U, Z) < \infty, \quad t \geq t_0, \quad U \in Y_*(t), \quad Z \in Z_*(t), \quad (2.17)$$

$$N_*(t, U, Z) = \int_{\Omega(t) \times \mathbb{R}^3} f_*(t, X, V, U, Z) dX dV, \quad t \geq t_0, \quad U \in Y_*(t), \quad Z \in Z_*(t), \quad (2.18)$$

function $f_*(t, \cdot, \cdot, U, Z)$, $t \geq t_0, U \in Y_*(t), Z \in Z_*(t)$ is the conditional distribution function conditioned with value $(U, Z)$ of variable $(u, z)$ at time $t$ and relation $z_*(\xi, t) = Z$.  

Features (2.16)–(2.19) generalize (2.2)–(2.5). Quantity (2.19) is the conditional number of the fluid particles in domain $\Omega(t)$ under the conditions that the value of variable $(u, z)$ at
time \( t \) is \( (U, Z) \) and \( z_*(\xi, t) = Z \). The probabilistic meaning of conditional distribution function \( f_*(t, \cdot, \cdot, U, Z) \) is described in the Appendix in connection with the stochastic process introduced in Section 4.1. The fact that \( f_*(t, \cdot, \cdot, U, Z) \) is conditioned with the values of both variables \( u \) and \( z \) enables one, in Section 5, to return to vector (2.7), however, in light of the new issues developed in Sections 3 and 4.

It follows from (2.20) and the probabilistic meaning of function \( \nu_*(t, u, \cdot) \) that

\[
\nu_*(t, x) = \int_{\mathbb{R}^3} f_*(t, x, u, z) \nu_*(t, u, z) \, dz,
\]

This means that the term \( f_*(t, x, u, z) \) in (2.21) generalizes the term \( f_*(t, x, u) \) in the integrand in (2.13). Subsequently, we replace (2.13) with (2.21).

This (see also Remark 2.4) in particular transforms (2.6) into

\[
f_*(t, x, u, z) = \int_{\mathbb{R}^3} \sum_{i=1}^M f_i(t, x, u, z, u_i, z) \nu_i(t, u_i, z) \, dz,
\]

This means that if \( U_1, \ldots, U_M \in Y_*(t) \) and functions \( f_i \) and \( \nu_i \) are known, then functions \( \varphi_{*,i}, \ldots, \varphi_{*,M} \) can be determined by means of (3.1).

Thus, the modelling of a multicomponent fluid in Section 2 leads to the GK approach. The new feature is the conditional structure of functions \( \varphi_{*,i}, \ldots, \varphi_{*,M} \), expressed in the form of (3.1) with

\[
\varphi_{*,i}(t, x, u, z) = \sum_{i=1}^M f_i(t, x, u, z) \nu_i(t, u_i, z),
\]

This means that if \( U_1, \ldots, U_M \in Y_*(t) \) and functions \( f_i \) and \( \nu_i \) are known, then functions \( \varphi_{*,1}, \ldots, \varphi_{*,M} \) can be determined by means of (3.1).

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\[
\varphi_{*,i}(t, x, u, z) = \sum_{i=1}^M f_i(t, x, u, z) \nu_i(t, u_i, z),
\]

This means that if \( U_1, \ldots, U_M \in Y_*(t) \) and functions \( f_i \) and \( \nu_i \) are known, then functions \( \varphi_{*,1}, \ldots, \varphi_{*,M} \) can be determined by means of (3.1).

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\varphi_{*,i}(t, x, u, z) = \sum_{i=1}^M f_i(t, x, u, z) \nu_i(t, u_i, z),
\]
4.1. The Continuum Generalization of the Total Generalized Distribution Function

The continuum generalization of the terms summed in (2.6) which was started from (2.10) has led, in Section 3, to the GK-theory expression (2.22). Let us examine what advantages can be granted by the continuum generalization of the summation in (2.22).

In the particular case as \( Y*(t) = l \), equality (2.22) can be rewritten as follows:

\[
\begin{align*}
    f(t, x, v) & = M \int_{\mathcal{Y}(t) \times \mathcal{Z}(t)} f(t, x, v, u, z) \nu(u) \nu(t, u, z) dU dZ, \\
    \quad M \geq 1, \quad t \geq t_0, \quad x \in \mathcal{O}(t), \quad v \in \mathbb{R}^3, \quad Y*(t) = \mathbb{R}^l, \quad Z \in \mathcal{Z}(t), \tag{4.1}
\end{align*}
\]

where

\[
\nu(U) = M^{-1} \sum_{i=1}^{M} \delta_i(U - U_i), \quad U_i, U \in Y*(t) \equiv \mathbb{R}^l, \tag{4.2}
\]

and \( \delta_i \) is the Dirac delta-function in \( \mathbb{R}^l \). Note that the delta-function expression (4.2) for \( \nu(U) \) in (4.1) does not incorporate additional limitations into (2.12) and (2.17). The point is that (4.1) is meaningful even if function \( f(t, x, v, u, z) \nu(t, u, z) \) is understood in the sense of the generalized functions since (e.g., [22, p. 123]) the convolution of any generalized function defined on \( \mathbb{R}^l \) with delta-function \( \delta_i \) exists and is equal to the very generalized function.

Function (4.2) is obviously a probability density. This enables one to apply the following probabilistic reading of the component-state vector variable \( u \). One can regard it as the random variable, say, \( u(\cdot) \) described with probability density \( \nu(\cdot) \) where \( u \) is a function of elementary event \( \xi \in \Xi \). Number \( M \) of the fluid components can be determined in terms of the density alone. Indeed, the \( i^{th} \) component of the fluid, \( i = 1, \ldots, M, \) is presented in (4.2) with the delta-function centered at \( U = U_i \), i.e., with the corresponding peak of \( \nu \). These peaks are the points of the strict local (or isolated) maximums of \( \nu \) at \( U = U_i \). The term "strict local" agrees with property (2.8). Abscissas \( U_1, \ldots, U_M \) are the modes of density \( \nu \) since the abscissa of any point of the local maximum of a probability density is called (e.g., [23, Chapter 15]) the mode of the density. Clearly,

\[
\text{number } M \geq 1 \text{ of the fluid components is the number of modes } U_1, \ldots, U_M \text{ of probability density (4.2).} \tag{4.3}
\]

Remark 4.1. The probabilistic vision provides a sharp interpretation of the fluid components. Indeed, every mode of the related probability density is the inherent manifestation of the component corresponding to this mode. This is the key feature that enables one to treat the set of the components as the set of the modes. The resulting conceptual advantage is the passing from the discrete objects, different groups of the fluid particles (see Section 2.1), to a certain, well-defined characteristic in the continuum paradigm, methodologically more general, flexible, and capable than the discrete, component-based approach.

Examples of multimodality can be found in population dynamics (e.g., [24]), physics (e.g., [25]), chemistry (e.g., [26]), catastrophe theory (e.g., [27-30]), and other sciences. The corresponding practical aspects and the related issues are also presented in a series of works (e.g., [31-33]).

Let function \( \nu_*(t, \cdot) \) of variable \( U \in Y_*(t) \) and quantities \( M_*(t), U_{1*}(t), \ldots, U_{M*}(t) \) be defined with the following properties.

Function \( \nu_*(t, \cdot), t \geq t_0, \) is a probability density. \( \tag{4.4} \)

Function \( \nu_* \) is sufficiently regular with respect to all its variables. \( \tag{4.5} \)

Quantity \( M_*(t) \), where \( M_* : [t_0, \infty) \rightarrow \{1, 2, \ldots\} \), is the number of the modes of probability density \( \nu_*(t, \cdot) \) at time \( t \geq t_0. \) \( \tag{4.6} \)
Vectors $U_{*,1}(t), \ldots, U_{*,M_*(t)}(t)$ are the modes of probability density $v_*(t, \cdot)$ at time $t \geq t_0$.

(4.7)

The modes in (4.7) are pairwise different at every fixed $t \geq t_0$

such that $M_*(t) > 1$, i.e., $U_{*,i}(t) \neq U_{*,j}(t)$, $i, j = 1, \ldots, M_*(t) : i \neq j$.

(4.8)

Now we replace $v(U)$, $M$, and $U_{1, \ldots, U_M}$ with $v_*(t, U)$, $M_*(t)$, and $U_{*,1}(t), \ldots, U_{*,M}(t)$, respectively. In particular, (2.14) and (2.15) become

(4.9)

number $M_*(t)$, $t \geq t_0$, can be on the order of tens or hundreds.

(4.10)

One of the corresponding results is expression

$$f_*(t, X, V) = \int_{Y_*(t) \times Z_*(t)} \varphi_*(t, X, V, U, Z) dU dZ, \quad t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3,$$

(4.11)

where

$$\varphi_*(t, X, V, Z) = M_*(t)f_*(t, X, V, U, Z)v_*(t, U)\nu_*(t, U, Z), \quad t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U \in Y_*(t), \quad Z \in Z_*(t).$$

(4.12)

Expression (4.11) generalizes (4.1). Function $\varphi_*$ in (4.11) is the single generalized distribution function for the whole multicomponent fluid. Definitions (4.6) and (4.7) extend (4.3). Feature (4.8) is the time-dependent version of (2.8).

Thus, the present modelling of a multicomponent fluid leads not only to the GK theory based on the generalized distribution functions for each component (see Section 3)), but also to an even more capable generalised function, $\varphi_*$, single for the whole fluid, no matter how many components the fluid includes. In so doing, the number of the components is determined with (4.6). Function $\varphi_*$ can be regarded as the overall generalised distribution function.

Definition (4.4) generalizes probability density $v$. Subsequently, random variable $u(\cdot)$ describing the component-state vector variable $u$ is extended to a stochastic process, say, $u_*(\cdot, \cdot)$, so $u = u_*(\xi, t)$. This, together with the description of the particle state $z$ by stochastic process $z_*$ introduced in Section 2.4, means that the particle-property vector variable (2.7) is modelled as follows:

$$q = q_*(\xi, t) = \left( u_*(\xi, t) \right), \quad t \geq t_0,$$

(4.13)

where $q_*(\cdot, \cdot)$ can be regarded as the particle-property stochastic process.

Let function $\rho_*(t, \cdot, \cdot)$ be determined with equality

$$\rho_*(t, U, Z) = v_*(t, U)\nu_*(t, U, Z), \quad t \geq t_0, \quad U \in Y_*(t), \quad Z \in Z_*(t).$$

(4.14)

Note that

$$\text{function } \rho_*(t, \cdot, \cdot), \quad t \geq t_0, \quad \text{is a probability density},$$

(4.15)

$$\text{function } \rho_*, \text{ is sufficiently regular with respect to all its variables},$$

(4.16)

because of (4.4), (4.5), (2.11), and (2.12). By virtue of (4.4) and (2.11), random variable $q_*(\cdot, t)$ (see (4.13)) is described with probability density (4.14). In terms of (4.14), densities $v_*(t, \cdot)$ and $\nu_*(t, U, \cdot)$ are interpreted in the following way. Density $v_*(t, \cdot)$ is the marginal probability density of random variable $u_*(\cdot, \cdot)$ in (4.14), whereas density $\nu_*(t, U, \cdot)$ is the conditional probability density of random variable $z_*(\cdot, t)$ under the condition that $u_*(\xi, t) = U$. They can be determined by means of $\rho_*(t, \cdot, \cdot)$, namely, with expression

$$v_*(t, U) = \int_{Z_*(t)} \rho_*(t, U, Z) dZ, \quad t \geq t_0, \quad U \in Y_*(t),$$

(4.17)
and from equality (4.14). In other words, $\rho_\ast(t, \cdot, \cdot)$ is the joint probability density of random variables $u_\ast(\cdot, t)$ and $z_\ast(\cdot, t)$ or, equivalently, the probability density of random variable

$$q_\ast(\cdot, t) = \begin{pmatrix} u_\ast(\cdot, t) \\ z_\ast(\cdot, t) \end{pmatrix}, \quad t \geq t_0. \quad (4.18)$$

Also note that (4.12) is, in terms of (4.14), rewritten as

$$\varphi_\ast(t, X, V, U, Z) = M_\ast(t)f_\ast(t, X, V, U, Z)\rho_\ast(t, U, Z),$$

$$t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U \in \mathbf{Y}_\ast(t), \quad Z \in \mathbf{Z}_\ast(t). \quad (4.19)$$

The probabilistic picture associated with multicomponent function $\varphi_\ast$ is considered in the next section.

### 4.2. The Probabilistic Meaning of the Overall Generalized Distribution Function

The probabilistic meaning of conditional distribution function $f_\ast(\cdot, \cdot, \cdot, U, Z)$ conditioned with value $Q$ (see (2.9)) of $q_\ast(\xi, t)$ (see (4.13)) is described in the Appendix. Combining (4.19) and (A.6), one obtains

$$\varphi_\ast(t, X, V, U, Z) = M_\ast(t)N_\ast(t, U, Z)\eta_\ast(t, X, V, U, Z),$$

$$t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U \in \mathbf{Y}_\ast(t), \quad Z \in \mathbf{Z}_\ast(t). \quad (4.20)$$

where

$$\eta_\ast(t, X, V, U, Z) = \zeta_\ast(t, X, V, U, Z)\rho_\ast(t, U, Z),$$

$$t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U \in \mathbf{Y}_\ast(t), \quad Z \in \mathbf{Z}_\ast(t). \quad (4.21)$$

It follows from the Appendix, the text around (4.11)-(4.18), as well as relations (4.20) and (4.21) that

- probability density $\rho_\ast(\cdot, \cdot, \cdot)$ (see (4.14)) is the probability density of random variable $q_\ast(\cdot, t)$ (see (4.13)) which is marginal with respect to random variable (A.8), and
- overall generalized distribution function $\varphi_\ast$ (see (4.20)) describes
  - number $M_\ast(t)$ (see (4.6)) of the components of the fluid;
  - conditional number $N_\ast(t, U, Z)$ (see (2.19) or (A.4)) of the fluid particles in domain $\Omega(t)$ under the condition that $q_\ast(\xi, t) = Q$;
  - vectors $x$, $v$, $u$, and $z$ of the particle position, particle velocity, component state, and particle state as stochastic processes, i.e., functions $x$, $v$, $u_\ast$, and $z_\ast$ of elementary event $\xi$ and $t$, i.e., $x = x(\xi, t)$, $v = v(\xi, t)$, $u = u_\ast(\xi, t)$, and $z = z_\ast(\xi, t)$; more specifically, density $\eta_\ast(t, \cdot, \cdot, \cdot, \cdot)$ (see (4.21)) is the joint probability density of random variables $x(\cdot, t)$, $v(\cdot, t)$, $u_\ast(\cdot, t)$, and $z_\ast(\cdot, t)$ for $t \geq t_0$ or, equivalently, the probability density of random variable (see (A.8) and (4.18))

$$\begin{pmatrix} x(\cdot, t) \\ v(\cdot, t) \\ u_\ast(\cdot, t) \\ z_\ast(\cdot, t) \end{pmatrix}.$$

This shows that the component- and particle-state vector variables $u = u_\ast(\xi, t)$ and $z = z_\ast(\xi, t)$ are modeled in equal terms with the particle position and velocity vectors $x = x(\xi, t)$ and $v = v(\xi, t)$. This is not achieved within the limits of common statistical-mechanics paradigm.
5. THE UNIFIED PICTURE: THE FULLY CONTINUUM ALTERNATIVE TO THE DISCRETE, COMPONENT-BASED STATISTICAL-MECHANICS VISION

It is clear from the picture in Section 4.2 that all the key quantities in the present analysis can be rewritten in terms of stochastic process \( q_\tau(\cdot, t) \) (see (4.13)) and its values \( Q \) (see (2.9)). Indeed, relations (4.11), (4.18), (2.16)-(2.20), (4.15), (4.16) become

\[
f_o(t, X, V) = \int_{K_\tau(t)} \varphi_\tau(t, X, V, Q) \, dQ, \quad t \geq t_\tau, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \tag{5.1}
\]

\[
\varphi_\tau(t, X, V, Q) = M_\tau(t) f_\tau(t, X, V, Q) \rho_\tau(t, Q), \quad t \geq t_\tau, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad Q \in K_\tau(t), \tag{5.2}
\]

\[
f_\tau(t, X, V, Q) \geq 0, \quad t \geq t_\tau, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad Q \in K_\tau(t), \tag{5.3}
\]

function \( f_\tau \) is sufficiently regular with respect to all its variables,

\[
0 < N_\tau(t, Q) < \infty, \quad t \geq t_\tau, \quad Q \in K_\tau(t), \tag{5.4}
\]

\[
N_\tau(t, Q) = \int_{\Omega(t) \times \mathbb{R}^3} f_\tau(t, X, V, Q) \, dX \, dV, \quad t \geq t_\tau, \quad Q \in K_\tau(t), \tag{5.5}
\]

function \( f_\tau(t, \cdot, \cdot, Q) \), \( t \geq t_\tau, Q \in K_\tau(t) \), is the conditional distribution function conditioned with value \( Q \) of \( q_\tau(\cdot, t) \),

function \( \rho_\tau(t, \cdot) \) of \( Q \in K_\tau(t) \), \( t \geq t_\tau \), is a probability density of the particle-property random variable \( q_\tau(\cdot, t) \),

function \( \rho_\tau \) is sufficiently regular with respect to all its variables,

respectively, where domain \( K_\tau(t) \subset \mathbb{R}^\kappa \) is expressed as

\[
K_\tau(t) = Y_\tau(t) \times Z_\tau(t), \quad Y_\tau(t) \neq \emptyset, \quad t \geq t_\tau, \tag{5.10}
\]

\[
\kappa = l + m, \quad l \geq 1, \quad m \geq 0. \tag{5.11}
\]

**Remark 5.1.** Comparison of (5.1) and (5.2) with (2.6) at \( M_\tau = M_\tau(t) \) shows that, at fixed \( t \geq t_\tau \), the multiplication by \( M_\tau(t) \rho_\tau(t, Q) \) with the subsequent integration in \( Q \) over \( K_\tau(t) \) is, loosely speaking, the continuum generalization of the discrete, index-based operation \( \sum_{i=1}^{M_\tau(t)} \).

All the quantities in the probabilistic reading of function \( f_\tau(t, \cdot, \cdot, Q) \) in the Appendix are easily represented completely in terms of the particle-property stochastic process \( q_\tau(\cdot, \cdot) \) and its value \( Q \) by means of (4.13) and (2.9). The only quantity which may seem to be impossible to interpret in terms of probability density (5.8) alone is \( M_\tau(t) \) in (5.2). Indeed, according to (4.6) (see also (4.7)), it is determined by means of probability density \( \upsilon_\tau(t, \cdot) \) for \( u \) that, in view of (4.17), is generally not the same as density (5.8) which, as is shown in (4.14), also includes conditional density \( \upsilon_\tau(t, U, \cdot) \) for \( z \). However, both \( u \) and \( z \) are (see (2.9)) vector-entries of vector \( q \) described by density \( \rho_\tau(t, \cdot) \). In so doing, vector \( z \), by its definition (see the first paragraph of Section 2.2), denotes the particle properties which do not affect the number of the fluid components or, following Remark 4.1, the number of the modes determined by vector \( u \). This means that probability densities \( \upsilon_\tau(t, \cdot) \) and \( \rho_\tau(t, \cdot) \) have the same number \( M_\tau(t) \) of the modes. Subsequently, features (4.6)-(4.8) are, in conjunction with Remark 4.1, reformulated as follows:

- scalar \( M_\tau(t) \) where \( M_\tau : [t_\tau, \infty) \to \{1, 2, \ldots\} \) is the number of the modes of probability density \( \rho_\tau(t, \cdot) \) at time \( t \geq t_\tau \) and \( \) the number of the "components" of the fluid described with (5.2);
Generalized Kinetic Modelling

vectors $Q_{*,1}(t), \ldots, Q_{*,M}(t)$ are the modes of probability density $\rho_*(t, \cdot)$ at time $t \geq t_o$ and these modes determine the "components" of the fluid described with (5.2);

the modes in (5.13) are pairwise different at every fixed $t \geq t_o$

such that $M_*(t) > 1$, i.e., $Q_{*,i}(t) \neq Q_{*,j}(t)$, $i, j = 1, \ldots, M_*(t)$ : $i \neq j$. (5.14)

If, in one or another specific problem, one needs the sharp continuum analogues of distribution functions $f_1, \ldots, f_{M_*(t)}(t)$ in (2.6) at $M_0 = M_*(t)$, then functions $f_\cdot(\cdot, \cdot; Q_{*,i}(t), t \leq t_o)$, $i = 1, \ldots, M_*(t)$, can be used in this capacity. Also note that the first inequalities in (5.10) and (5.11) concern only the $u$-related terms. This means that vector entry $z$ (and $Z$) of vector $q$ (and $Q$) (see (2.7), (2.9)) may be absent. In the latter case, the number of the modes is determined with all the entries of vector $q$, i.e., all the properties of the fluid particles, and, subsequently, $m = 0, \kappa = \ell$, $K_*(t) = Y_*(t)$, and $Z_*(t) = \emptyset$.

Relations (5.12)-(5.14) point out that the component content of the modelled multicomponent fluid is fully determined by the time-evolution of the number of the modes, i.e., the abscissas of the strict-local-maximum points of the probability density, and the shapes and relative heights of the maximum peaks. The quotation marks in (5.12) and (5.13) stress that the component-based vision (see Section 2.1 and Remark 4.1) is no longer used in this work. They point out the historical origin of the present, modality-based treatment. This treatment provides a modelling framework which can resolve many problems listed in Remark 2.1. For instance, number $M_*(t)$ of the modes of the time-dependent probability density naturally depends on time and results from the evolution of the density that models the evolution of the particle properties. In so doing, there are generally no sharp borders between the "components" in line with the actual nature of the real-life fluids. The modes are dynamically varied in the course of the evolution, become more or less pronounced, can disappear and appear depending on a specific nature of the fluid and the external excitations. The mode landscape can be complicated even in the time-independent, stationary case (e.g., see the examples in [27, Figures 2 and 4; 28, Figure 2; 30, Figure 1]). The diversity of the mode-related alterations is virtually infinite.

Remarkably, the above flexibility is provided by a single generalized distribution function. Indeed, overall generalized distribution function $\varphi_{*,M}$ (see (5.2)) is very similar to any of $\varphi_{*,1}, \ldots, \varphi_{*,M}$ in Section 3. More precisely, if $M_*(t) = 1$ at fixed $t \geq t_o$, then (5.2) at this $t$ is the same as the generalized distribution function for one-component fluid in the GK treatment (e.g., see function $f$ in [10, Section 3] or $f$ in [11, Section 2]). In this case, probability density $\rho_*(t, \cdot)$ at the above $t$ has exactly one mode. (If, in so doing, probability density $\rho_*(t, \cdot)$ does not have a mode, then vector $q$ (see (2.7)) does not include vector entry $u$ (see also the text below (5.14)), the first inequalities in (5.10) and (5.11) are violated, and the model must be revised, respectively.) If $M_*(t) > 1$ at fixed $t \geq t_o$, then (5.2) at this $t$ differs from the one-component version of (5.2) only with multiplier $M_*(t)$. In this case, probability density $\rho_*(t, \cdot)$ at the above $t$ has exactly $M_*(t)$ modes (note (4.9) and (4.10) for biological fluids).

These issues show that the overall generalized distribution function (5.2) can be regarded as the natural multimodal (or "multicomponent") extension of the one-component generalized distribution function in the GK theory.

6. MODELLING OF THE OVERALL GENERALIZED DISTRIBUTION FUNCTION

Total distribution function $f_0$ is described with (5.1) by means of overall generalized distribution function $\varphi_{*,*}$. Modelling of the latter can be based on representation (5.2). According to it, it is sufficient to model conditional distribution function $f_\cdot$ and probability density $\rho_*$. In so doing, quantity $M_*(t)$ is determined as is pointed out in (5.12).
Functions \( f_* \) and \( \rho_* \) are scalar, and hence, can be described with a system of two appropriate scalar equations. Sections 6.1 and 6.2 below consider possible versions of these equations. Section 6.1 outlines a generalized kinetic equation for conditional distribution function \( f_* \), whereas Section 6.2 discusses

(i) a system of McKean-Itô's stochastic differential equations, McKean ISDEs (MISDEs), for the particle-property stochastic process \( q_* \), and
(ii) the corresponding McKean-Kolmogorov forward equation, McKean KFE (MKFE), for probability density \( \rho_* \) describing \( q_* \).

6.1. A Generalized Kinetic Equation for the Conditional Distribution Function

To get an idea on a general structure of a kinetic equation for conditional distribution function \( f_* \), we come back for a while to common, component-based vision in Section 2.1. In this treatment, distribution functions \( f_1, \ldots, f_{M_0} \) are usually described with the following kinetic-equation system:

\[
\begin{align*}
\frac{\partial f_i(t, X, V)}{\partial t} + \sum_{j=1}^{3} \frac{\partial f_i(t, X, V)}{\partial X_j} V_j + \sum_{j=1}^{3} \frac{\partial f_i(t, X, V)}{\partial V_j} a_{i,j}(t, X, V) & = J_{i,0}(t, X, V, f_i(t, X, \cdot)) + \sum_{j=1}^{M_0} J_{ij}(t, X, V, f_i(t, X, \cdot), f_j(t, X, \cdot)), \\
M_0 & \geq 1, \quad i = 1, \ldots, M_0, \quad t > t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3,
\end{align*}
\]  

(6.1)

where scalars \( X_j, V_j, \) and \( a_{i,j}(t, X, V) \) are the entries of vectors \( X, V, \) and \( a_i(t, X, V) \), respectively, and vector \( a_i(t, X, V) \) is the acceleration of the particle of the \( i^{th} \) component because of the external forces acting on the particle. The terms on the right-hand side of (6.1) are called collision terms. Scalar \( J_{i,0}(t, X, V, f_i(t, X, \cdot)) \) is due to the collisions of the particles of the \( i^{th} \) component with the surrounding medium, whereas scalar \( J_{ij}(t, X, V, f_i(t, X, \cdot), f_j(t, X, \cdot)) \) is due to the inter-particle collisions, i.e., the collisions of the particles of the \( i^{th} \) component with the particles of the \( j^{th} \) component. The meaning of the interparticle collision terms \( J_{ij}(t, X, V, f_i(t, X, \cdot), f_j(t, X, \cdot)) \) implies that

\[
J_{ij}(t, X, V, f_i(t, X, \cdot), f_j(t, X, \cdot)) = J_{ji}(t, X, V, f_j(t, X, \cdot), f_i(t, X, \cdot)), \quad M_0 \geq 2, \quad i, j = 1, \ldots, M_0, \quad i \neq j, \quad t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3.
\]  

(6.2)

There is a great variety of kinetic equations (e.g., [4,8,34–36]) depending on the specific forms of the above collision terms. Following the reasoning similar to that in Sections 2–5 (in particular, Remark 5.1), one can suggest the following generalized kinetic equation:

\[
\begin{align*}
\frac{\partial f_*(t, X, V, Q)}{\partial t} & + \sum_{i=1}^{3} \frac{\partial f_*(t, X, V, Q)}{\partial X_i} V_i + \sum_{i=1}^{3} \frac{\partial f_*(t, X, V, Q)}{\partial V_i} a_*(t, X, V, Q) \\
& = J_{*,0}(t, X, V, Q, f_*(t, X, \cdot)) + \int_{K_*(t)} J_*(t, X, V, Q, f_{*,}(t, X, \cdot, Q), P, f_{*,}(t, X, \cdot, P)) \rho_*(t, P) dP, \\
\end{align*}
\]  

(6.3)

for conditional distribution function \( f_* \). In this equation, vector function \( a_*(t, \cdot, \cdot, Q) \) (with entries \( a_{*,j}(t, \cdot, \cdot, Q) \) where \( Q \) varies in \( K_*(t) \)) is the continuum analogue of vectors \( a_i(t, \cdot, \cdot) \) in (6.1) where \( i \) varies in \( \{1, \ldots, M_0\} \). Function \( J_{*,0}(t, \cdot, \cdot, Q, f_{*,}(t, \cdot, \cdot, Q)), Q \in K_*(t), \) in (6.3) is the corresponding extension of the function set \( J_{i,0}(t, \cdot, \cdot, f_i(t, \cdot, \cdot)), i = 1, \ldots, M_0, \) in (6.1). The function set \( J_{ij}(t, \cdot, \cdot, f_i(t, \cdot, \cdot), f_j(t, \cdot, \cdot)), i, j = 1, \ldots, M_0, \) in (6.1) is generalized with function
Generalized Kinetic Modelling

The latter, together with (6.2), points out that the property

\[ J_e(t, X, V, Q, f_e(t, X, V, Q), P, f_e(t, X, V, P)) = J_e(t, X, V, P, f_e(t, X, V, P), Q, f_e(t, X, V, Q)), \]

\[ t \geq t_o, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad Q, P \in K_(t), \quad Q \neq P. \]

must hold. The first and second terms on the right-hand side of (6.3) are related to the particle collisions with the surrounding medium and the interparticle collisions, respectively.

To specify the unique solution of equation (6.3), one supplies it with appropriate

(i) boundary conditions at the boundaries of domains \( \Omega(t) \) and \( \mathbb{R}^3 \) of variables \( X \) and \( V \) (which in particular comprise (2.16), (2.18), and (2.19) with notation (2.9)), and

(ii) conditions at the initial time point \( t = t_o \).

Usually, the corresponding initial-boundary problem is uniquely solvable only under certain regularity conditions, so function \( \rho_e \) in (6.3) and solution \( f_e \) of (6.3) are in a certain sense "well behaving". This feature was anticipated in (2.17) and (5.9).

Note that generalized kinetic equation (6.3) does not include the partial derivatives of conditional distribution function \( f_e(t, \cdot, \cdot, Q) \) with respect to entries of vector \( Q \), since (see (5.7)), this function is conditioned with value \( Q \) of \( q_e(t, \cdot) \). The \( Q \)-dependence of \( f_e(t, \cdot, \cdot, Q) \) in (6.3) is determined with the explicit \( Q \)- and \( P \)-dependencies of \( J_e \) and \( J_a \). These facts and the \( \rho_e \)-based integral form of the above interparticle-collision term in (6.3) are the features which somewhat differ the present generalized kinetic equations for the conditional distribution functions from the generalized kinetic equations for the generalized distribution functions in the GK theory [9, Section 10.3; 10, 11].

The form of the right-hand side of (6.3) shows that solution \( f_e(t, X, V, Q) \) at each \( V \in \mathbb{R}^3 \) is coupled with \( f_e(t, X, \cdot, Q) \), i.e., with the solution values for all \( V \in \mathbb{R}^3 \). This nonlocality is, however, a generic feature of kinetic equations. Remarkably, the above interparticle-collision term means that solution \( f_e(t, X, V, Q) \) at each \( Q \in K_(t) \) is coupled with \( f_e(t, X, V, P) \) for all \( P \in K_(t) \), thereby providing one more nonlocal (or "mean-field") effect in generalized kinetic equation (6.3) making it doubly nonlocal (in both \( V \) and \( Q \)). This is in line with the mean-field development of [10]. The interparticle-collision term in (6.3) is also discussed in the next section in connection with the MKFE model for probability density \( \rho_e \) involved in this term.


McKean-Kolmogorov's Forward Equation for the Probability Density

The last paragraph of Section 5 of [11] points out that, in terms of the present work, the particle-property stochastic process \( q_e \), can be described with a system of stochastic evolution equations. We consider a particular type of these equations, namely, MISDEs [37,38]. Systems of MISDEs generalize the well-known ISDE system (e.g., [39]) to the nonlocal effects and provide (under rather mild conditions) probability density \( \rho_e \) as a solution of the corresponding MKFE. Moreover, the ISDE-based descriptions in connection with the multimodal densities determined from KFEs are well known due to the works of Cobb (e.g., [27–30]).

Following this line, we model the particle-property stochastic process \( q_e \), as the solution \( q = q_e(t, \cdot, \cdot) \) of the following MISDE system:

\[ dq = g_e(t, q, f_e(t, \cdot, \cdot), \rho_e(t, \cdot)) dt + h_e(t, q, f_e(t, \cdot, \cdot), \rho_e(t, \cdot)) dW(\xi, t), \quad t > t_o, \]

\[ \lim_{t \to t_o} q_e(\cdot, t) = q_{e-o}(\cdot), \]

with initial condition
where \( q_{*,0}(\cdot) \) is the initial random variable described with the initial probability density \( \rho_{*,0}(\cdot) \). Probability density \( \rho_* \) in (6.5) (and (6.3)) is, as before, the probability density of random variable \( q_{*}(\cdot,t) \) of solution \( q = q_{*}(\cdot,\cdot) \) of initial-value problem (6.5),(6.6). Thus, MISDE system (6.5) can be viewed as the ISDE system where the solutions, stochastic processes, are coupled with the probability density describing them. Note that stochastic, ISDE or MISDE, descriptions are in line with Point (c) in Section 1.

**Remark 6.1.** Variable vector \( q \) in (6.5) (represented with variable vector \( Q \) in (6.3)) is in domain \( K_*(t) \) (see (5.10)) that generally need not coincide with the entire space \( \mathbb{R}^\kappa \) (see (5.11) for \( \kappa \)). Assume that, by means of a proper nonlinear change of variable \( q \) and application of the well-known Itô formula (e.g., [39, (5.3.11)]), MISDE system (6.5) can be transformed into a similar MISDE system but defined on \( \mathbb{R}^\kappa \). Then, without a loss of generality (more specifically, up to a change of the variable), (6.5) can be regarded as the very system on \( \mathbb{R}^\kappa \) and, thus, \( q \in \mathbb{R}^\kappa \) in (6.5). In this case, common theory of ISDEs and diffusion stochastic processes can be used. In particular, an analytical basis of the combined, analytical-numerical methods, efficient for the case when dimension \( \kappa \) is much greater than a few units can be found in [40].

We shall follow the entire-space convention in this remark down to the end of Section 7. Since so, probability density \( \rho_* \) is described (e.g., [39, (9.3.1)]) as the solution of MKFE

\[
\frac{\partial \rho_*(t,Q)}{\partial t} = -\sum_{i=1}^{\kappa} \frac{\partial}{\partial Q_i} \left[ g_{*,i}(t,Q,f_*(t,\cdot,\cdot,\cdot),\rho_*(t,\cdot))\rho_*(t,Q) \right] + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2}{\partial Q_i \partial Q_j} \left[ H_{*,ij}(t,Q,f_*(t,\cdot,\cdot,\cdot),\rho_*(t,\cdot))\rho_*(t,Q) \right],
\]

\( t > t_0, \quad Q \in \mathbb{R}^\kappa \),

with the probability-density condition (5.8) and initial condition

\[
\lim_{t \downarrow t_0} \rho_*(\cdot,t) = \rho_{*,0}(\cdot),
\]

where

\[
H_{*,ij}(t,Q,f_*(t,\cdot,\cdot,\cdot),\rho_*(t,\cdot)) = h_{*,i}(t,Q,f_*(t,\cdot,\cdot,\cdot),\rho_*(t,\cdot),\rho_*(t,\cdot))\rho_*(t,\cdot) | h_{*,j}(t,Q,f_*(t,\cdot,\cdot,\cdot),\rho_*(t,\cdot))\rho_*(t,\cdot) |^T,
\]

\( t \geq t_0, \quad Q \in \mathbb{R}^\kappa \),

and functions \( g_{*,i} \) and \( H_{*,ij} \) are the entries of drift vector-function \( g_* \) and diffusion matrix-function \( H_* \), respectively. Since these functions depend on \( \rho_* \), MKFE (6.7) is nonlinear. (If both drift function \( g_* \) and diffusion function \( H_* \) are independent of \( \rho_* \), MKFE (6.7) becomes linear, i.e., common KFE. In this case, MISDE system (6.5) becomes a common ISDE system.)

Usually, the corresponding problem (6.7), (6.8), and (5.8) is uniquely solvable only under certain regularity conditions, so function \( f_* \) in (6.7) and solution \( \rho_* \) of (6.7) are in a certain sense “well behaving”. This feature was anticipated in (2.17) and (5.9).

The form of the right-hand side of (6.7) shows that solution \( \rho_*(t,Q) \) at each \( Q \in \mathbb{R}^\kappa \) is coupled with \( \rho_*(t,\cdot) \), i.e., with the solution values for all \( Q \in \mathbb{R}^\kappa \). This provides the nonlocal effect in (6.7). If one regards equation (6.7) as the one for, say, intrinsic evolution of \( \rho_* \), then the \( f_* \)-dependence of \( g_\cdot \) and \( H_\cdot \) can be read as an external action (cf. [10, Point (v) of Section 9]).

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The ISDE-based models where the drift and diffusion characteristics (see functions \( g_\cdot \) and \( h_\cdot \) in (6.5) or (6.7),(6.9)) are assumed to be sufficiently regular (e.g., [39, Section 9.3]), in particular, continuous describe the processes that are the diffusion ones, and hence, (e.g., [39, (2.5.1)]) continuous. However, results of [41] point out that the ISDE systems can sometimes model jump stochastic processes if \( g_\cdot \) or \( h_\cdot \) are discontinuous. This option applied to (6.7) can be helpful in connection with the jump-process topic in the GK theory (e.g., [10, Point (ii) of Section 9]).
Regarding the jump-process vision, we note that there are many real-life phenomena which are difficult (if possible at all) to model in this way. For instance, the well-known Heisenberg uncertainty principle points out that finite jumps of the particle energy cannot be instantaneous. In other words, the energy can switch from one finite value to another finite value only during a non-zero time interval. The same is also true for any other time evolution which include the energy "jumps" as the necessary conditions. The consequences of Heisenberg's uncertainty principle are fairly far reaching. In particular, it leads to the fundamental limits even for the quantities that are not directly related to quantum mechanics (e.g., [42]).

6.3. The Combined, Generalized-Kinetics/Nonlocal-Stochastics Model for the Overall Generalized Distribution Function

Sections 6.1 and 6.2 are devoted to the models for the following two parts of overall generalized distribution function \( \varphi_{\cdot} \) (see (5.2)): conditional distribution function \( f_{\cdot} \) and the corresponding probability density \( \rho_{\cdot} \). These models are generalized kinetic equation (6.3) and MKFE (6.7). They present a system of two coupled scalar equations. Thus, overall function \( \varphi_{\cdot} \) involved in (5.1) is described with expression (5.2) and the system of two scalar equations (6.3), (6.7), and condition (5.12) for \( f_{\cdot} \), \( \rho_{\cdot} \), and \( M_{\cdot} \), respectively, in (5.2), no matter how many "components" the modelled fluid include. Note that the nonlocal (or "mean-field") nature of (6.3) and (6.7) (see Sections 6.1 and 6.2) contributes to Point (b) in Section 1 and complements the mean-field research in [10].

Prescription (5.12) in connection with equation (6.7) for probability density \( \rho_{\cdot} \) is discussed in Section 7. In the present section, we only note the memory effect in system (6.3),(6.7). Indeed, as is explicitly shown by the forms of these equations, they are coupled. In so doing, function \( \rho_{\cdot} \) in equation (6.3) for \( f_{\cdot} \) (see the second, interparticle-collision term on the right-hand side) is determined from the time-evolution equation (6.7) that creates the memory effect (i.e., the extra relaxation) in \( f_{\cdot} \). This effect is absent if (6.3) is independent of \( \rho_{\cdot} \). Similarly, function \( f_{\cdot} \) in equation (6.7) for \( \rho_{\cdot} \) is determined from the time-evolution equation (6.3) that creates the memory effect (the extra relaxation) in \( \rho_{\cdot} \). This effect is absent if (6.7) is independent of \( f_{\cdot} \). Thus, model (6.3),(6.7) enriches the dynamics of \( f_{\cdot} \) and \( \rho_{\cdot} \) with the coupling of the time evolutions of these quantities. This memory effect answers the development direction outlined in [10, Point (iv) of Section 9].

7. MULTIMODALITY OF THE PARTICLE-PROPERTY PROBABILITY DENSITY IN THE GENERIC STATIONARY CASE

Regarding (5.12), one can note the following. Nowadays, determination of the number of the modes of the probability densities described with KFEs or MKFEs is not the most developed part of theory of stochastic processes and stochastic differential equations even in the one-dimensional case, i.e., when \( \kappa = 1 \), not to mention the multidimensional case or the high-mode-number case (4.10). The present section extends some aspects of Cobb's multimodality treatment [27-30] of one-dimensional stationary densities to the multidimensional ones. More specifically, it proposes a criterion formulated in terms of drift and diffusion functions \( g_{\cdot} \) and \( H_{\cdot} \) for any regular (in a certain sense) point in \( \mathbb{R}^\kappa \) to be a mode of probability density \( \rho_{\cdot} \).

In the stationary case, both functions \( f_{\cdot} \) and \( \rho_{\cdot} \) are independent of \( t \). Functions \( g_{\cdot} \) and \( h_{\cdot} \) in (6.5) or (6.7), and hence, function \( H_{\cdot} \) (see (6.9)) are also independent of \( t \). For the sake of simplicity, we assume that \( g_{\cdot} \), \( h_{\cdot} \), and \( H_{\cdot} \) are independent of \( \rho_{\cdot}(t, \cdot) \) and function \( f_{\cdot} \) is known, denote \( \tilde{g}_{\cdot}(Q) = g_{\cdot}(Q, f_{\cdot}(. , . , .)), \tilde{h}_{\cdot}(Q) = h_{\cdot}(Q, f_{\cdot}(. , . , .)), Q \in \mathbb{R}^\kappa, \)

\[
H_{\cdot}(Q) = h_{\cdot}(Q) [h_{\cdot}(Q)]^T, \quad Q \in \mathbb{R}^\kappa, \tag{7.1}
\]

and consider a fairly generic case formulated in the hypothesis of the theorem below.
THEOREM 1. Let the following conditions hold.

(a) \( \mathbf{g}_* \in C^1(\mathbb{R}^\kappa) \) and \( h_* \in C^2(\mathbb{R}^\kappa) \).

(b) Vector \( \mathbf{F}_*(Q) \) is the Fichera drift vector (e.g., [40, p. 54]), i.e., the \( \kappa \)-vector with entries \( \mathbf{F}_*,i(Q) \) determined as

\[
\mathbf{F}_*,i(Q) = g_*,i(Q) - \sum_{j=1}^{\kappa} \frac{\partial \mathbf{H}_*,ij(Q)}{\partial Q_j}, \quad i = 1, \ldots, \kappa, \quad Q \in \mathbb{R}^\kappa, \quad (7.2)
\]

where \( g_*,i(Q), \) and \( \mathbf{H}_*,ij(Q) \) are the entries of vector \( \mathbf{g}_*(Q) \) and matrix \( \mathbf{H}_*(Q) \) (see (7.1)).

(c) Scalar \( \Phi_*(Q) \) is the divergence of vector \( \mathbf{F}_*(Q) \), i.e.,

\[
\Phi_*(Q) - \sum_{i=1}^{\kappa} \frac{\partial \mathbf{F}_*,i(Q)}{\partial Q_i}, \quad Q \in \mathbb{R}^\kappa. \quad (7.3)
\]

(d) Matrix \( \mathbf{h}_*(Q) \) is nonsingular for all \( Q \in \mathbb{R}^\kappa \).

(e) Matrix \( \frac{\partial (\mathbf{H}_*(Q))^{-1}\mathbf{F}_*(Q)}{\partial Q} \) is symmetric for all \( Q \in \mathbb{R}^\kappa \).

(f) Probability density \( \rho_* \) is the unique solution of the detailed-balance equation (DBE) system (e.g., see [40, (1.12.13), (1.12.5), (1.126)]),

\[
\frac{1}{2} \sum_{j=1}^{\kappa} \mathbf{H}_*,ij(Q) \frac{\partial \rho_*(Q)}{\partial Q_j} = \mathbf{F}_*,i(Q)\rho_*(Q), \quad i = 1, \ldots, \kappa, \quad Q \in \mathbb{R}^\kappa. \quad (7.4)
\]

(g) If \( \rho_* \in C^2(\mathbb{R}^\kappa) \), then point \( Q_* \in \mathbb{R}^\kappa \) is any point which is regular in the sense that matrix \( \frac{\partial^2 \rho_*(Q)}{\partial Q^2} \) is nonzero.

Then the following assertions are valid.

(a) \( \rho_* \in C^2(\mathbb{R}^\kappa) \) and matrix \( \mathbf{H}_*(Q) \) is positive definite for all \( Q \in \mathbb{R}^\kappa \).

(b) If point \( Q_* \) is the abscissa of a strict local maximum (minimum) of probability density \( \rho_* \), then \( \rho_*(Q_*) > 0, \mathbf{F}_*(Q_*) = 0, \) and \( \Phi_*(Q_*) < 0(\Phi_*(Q_*) > 0) \).

(c) The number of the modes of probability density \( \rho_* \) is not less than the total number of the strict local maximums each of which can be regarded as a maximum in Assertion (b).

PROOF. The proof is not very difficult since it is based on the well-known results. We only point out the following two aspects. First, Assumption (e) is known (e.g., [40]) as the detailed-balance condition. It assures that DBE (7.4) is solvable. Second, the statements on the signs of \( \Phi_*(Q_*) \) in Assertion (b) can be obtained by means of

(i) the differentiation of the DBE system (7.4) with respect to \( Q_i, i = 1, \ldots, \kappa, \)
(ii) allowing for (7.3), and
(iii) subsequent substitution \( Q = Q_* \) into the resulting equality.

This gives

\[
\Phi_*(Q_*)\rho_*(Q_*) = \frac{1}{2} \text{tr} \left\{ \mathbf{H}_*(Q_*) \left[ \frac{\partial^2 \rho_*(Q_*)}{\partial Q^2} \right] \right\},
\]

where \( \text{tr}(\cdot) \) is the trace of matrix and the matrix of the second derivatives is mentioned in Assumption (g) and Assertion (a).

Assertion (c) of this theorem provides an estimation for \( M_*(t) \) in (5.12) in the stationary case. The theorem attracts attention to the Fichera drift vector (7.2) and its divergence (7.3). Indeed, according to Assertion (c), the modes of probability density \( \rho_* \) should be sought among the roots of equation \( \Phi_*(Q) = 0. \) In so doing, the roots that make \( \Phi_*(Q_*) \) negative can be the modes.

Theorem 1 includes helpful issues for development of the particle-property models (in the sense of Remark 6.1) which include the multimodality and a lower bound for the mode number in (5.12) at least in the above generic version of the stationary case. A lot of work is to be done to extend this approach to the general, time-dependent model (6.3), (6.7), and (5.12).
8. SUMMARY OF THE PROPOSED MODELLING AND DIRECTIONS FOR FUTURE RESEARCH

In statistical mechanics, the fluid total distribution function $f$, is described by (2.6), where $M_o$ is the number of the fluid components. This leads to a system of $M_o$ kinetic equations for the fluid-component distribution functions (e.g., (6.1)). For biological fluids, $M_o$ is very high in the sense of (2.1) (see also Remark 2.2).

Summing up this work, we note the following main result. In contrast to the above statistical-mechanics picture, the work describes $f$, with (5.1) (rather than (2.6)) where the overall generalized distribution function (5.2) is modelled with

- the system of two scalar equations, generalized kinetic equation (6.3) for the conditional distribution function conditioned with the values of the particle-property stochastic process and MKFE (6.7) for the particle-property probability density, and
- prescription (5.12) where number $M_s(t)$ of the density modes, or the fluid "components", is noticeably less than $M_o$ (see (4.9)); condition (5.12) includes the mode interpretation (5.13) of the "components" in terms of pairwise different modes (5.14).

Importantly, the mode number $M_s(t)$ is, according to (5.12), determined self-consistently in the course and terms of the time-evolution of the fluid. Theorem 1 in Section 7 provides an estimation from below for this number in the generic stationary case of the corresponding Kolmogorov equation and points out how the modes manifest themselves in the drift and diffusion functions (more specifically, in the Fichera drift function).

In connection with the above model, we suggest the following five directions for future research.

(i) Examples of the model for specific biological fluids not only will be of a practical importance but also will help to specify the formulation procedure for the terms of the model, in particular, functions $J_{*,w}$, $J_s$, $g_*$, and $h_*$. In so doing, the GK theory results can be used for the specification of equation (6.3) for the conditional distribution functions. In contrast to this, the specification of MKFE (6.7) for the particle-property probability density is a more challenging problem. The point is that equations for properties of the fluid particles are not very common. We are not sure that even modern chemistry and physics would immediately suggest any sharp recipes. A better subject-specific understanding will be highly valuable.

(ii) The latter topic is likely inherently associated with development of the general methodology for the formulation of the particle-property stochastic equations and its connection to the corresponding experimental data. This in particular includes the allowing for the particle internal degrees of freedom (see [43,44] for an example of the related statistical-mechanics treatment).

(iii) In spite of the methodological advantages of recipe (5.12), it is technically not very simple. Indeed, what procedure can evaluate the mode number $M_s(t)$ in (5.12) in case (4.10)? It seems that a lot of research on this topic has to be done: to our knowledge, no ready-to-use procedure is known nowadays in probability theory. In this field, one of the directions can be generalization of the estimation and other results of Theorem 1 (see Section 7) for the nonstationary case of MKFE (6.7) or at least of its linear in $p_*$, KFVE version. The above procedure may also concern novel, extended definitions of the modes of probability densities. This may be caused by various reasons. One of them can be the following. Under some conditions, for example, at the highly nonequilibrium states, the strict local maximums of density $p_*$ can become very smoothed, not pronounced at all. In fact, they will (at least during certain time intervals) not be the local maximums, but instead, will become hidden. In so doing, their abcissas, the modes of the density, can manifest themselves as a kind of "quasiexpections" of the density. However, at present, the probability-theory scenarios to treat this topic seems to be unclear.
(iv) A version of the fully continuum, multimodal/"multicomponent" model (6.3), (6.7), (5.12) can also be developed as a generalization of NNSHD [12,13]. The corresponding specific treatment would be of both practical and theoretical interest, also better elucidating the principles shared by the generalized kinetics and NNSHD. The particle-property stochastic process would considerably widen the NNSHD capabilities. On the other hand, an extension of the GK theory to the stochastic generalized kinetic equations would bring this theory to a new level of universality.

(v) How do we computationally implement all the above advances in a practically acceptable way? The nonlinear nonlocal system (6.3),(6.7) in conjunction with the multimodal recipe (5.12) under condition (4.10) is not a very simple problem from the computing viewpoint. We believe that, in this field, the combined, analytical-numerical kinetics-stochastics methods partly exemplified with the development in [40] can be helpful.

The model proposed in this work leads to a series of interesting problems in many areas including probability theory, generalized kinetic and stochastic differential equations, scientific and engineering computing in conjunction with biology, chemistry, and physics.

APPENDIX

THE PROBABILISTIC MEANING OF CONDITIONAL DISTRIBUTION FUNCTION

Conditional distribution function \( f(\cdot, \cdot, \cdot, U, Z) \) (see (2.20)) inherits the basic features of any of common distribution functions \( f_1, \ldots, f_M \). The probabilistic meaning of \( f(\cdot, \cdot, \cdot, U, Z) \) follows from (2.16)-(2.19).

By virtue of (2.20), quantity

\[
n_*(t, X, U, Z) = \int_{\mathbb{R}^m} f_*(t, X, V, U, Z) dV, \quad t \geq t_0, \quad X \in \Omega(t), \quad U \in Y_*(t), \quad Z \in Z_*(t), \quad (A.1)
\]

is the conditional concentration (or the particle-number volumetric density) of the fluid particles. In view of (A.1) and (2.16), one gets

\[
n_*(t, X, U, Z) \geq 0, \quad t \geq t_0, \quad X \in \Omega(t), \quad U \in Y_*(t), \quad Z \in Z_*(t). \quad (A.2)
\]

Relations (2.16), (A.1), and (A.2) point out that function \( \mu_*(t, \cdot, U, Z) \) determined by equality

\[
f_*(t, X, V, U, Z) = n_*(t, X, U, Z) \mu_*(t, X, V, U, Z), \quad t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U \in Y_*(t), \quad Z \in Z_*(t), \quad (A.3)
\]

is the conditional probability density of the particle-velocity vector \( v \) conditioned with value \( X \) of the particle-position vector \( x \) and value \( Q \) (see (2.9)) of vector \( q_*(\xi, t) \) (see (4.13)). (Vectors \( x \) and \( v \) are pointed out in the text above (2.2).) The \( (t, X, U, Z) \)-dependence of \( \mu_\cdot \) is due to the \( (t, X, U, Z) \)-dependence of both \( f_\cdot(t, \cdot, \cdot, U, Z) \) and \( n_\cdot(t, X, U, Z) \) in (A.3).

In view of (A.1), quantity \( N_*(t, U, Z) \), the conditional number of the fluid particles in domain \( \Omega(t) \) introduced with (2.19), can also be described with conditional-concentration function \( n_\cdot(t, \cdot, U, Z) \), namely,

\[
N_*(t, U, Z) = \int_{\Omega(t)} n_\cdot(t, X, U, Z) dX, \quad t \geq t_0, \quad U \in Y_*(t), \quad Z \in Z_*(t). \quad (A.4)
\]

Relations (2.18), (A.2), and (A.4) mean that function \( \lambda_*(t, \cdot, U, Z) \) determined by equality

\[
n_\cdot(t, X, U, Z) = N_*(t, U, Z) \lambda_\cdot(t, X, U, Z), \quad t \geq t_0, \quad X \in \Omega(t), \quad U \in Y_*(t), \quad Z \in Z_*(t), \quad (A.5)
\]
is the conditional probability density of the particle-position vector $x$ under the condition that $q_*(\xi, t) = Q$ (see (4.13) and (2.9)). The $(t, U, Z)$-dependence of $\lambda_*$ is due to the $(t, U, Z)$-dependence of both $n_*(t, \cdot, U, Z)$ and $N_*(t, U, Z)$ in (A.5).

Combining (A.3) and (A.5), one obtains

$$f_*(t, X, V, U, Z) = N_*(t, U, Z)\zeta_*(t, X, V, U, Z),$$

$$t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U \in Y_*(t), \quad Z \in Z_*(t),$$

where

$$\zeta_*(t, X, V, U, Z) = \lambda_*(t, X, U, Z)\mu_*(t, X, V, U, Z),$$

$$t \geq t_0, \quad X \in \Omega(t), \quad V \in \mathbb{R}^3, \quad U \in Y_*(t), \quad Z \in Z_*(t).$$

Function $f_*(\cdot, \cdot, U, Z)$ (see (A.6)) describes

- conditional number $N_*(t, U, Z)$ (see (2.18)) of the fluid particles in domain $\Omega(t)$, and
- vectors $x$ and $v$ of the particle position and velocity as stochastic processes, i.e., as functions $x$ and $v$ of elementary event $\xi$ and time $t$, $x = x(\xi, t)$ and $v = v(\xi, t)$; this description is conditioned with value $Q$ of vector $q_*(\xi, t)$ (see (2.9) and (4.13)).

In so doing, probability density $\zeta_*(t, \cdot, U, Z)$ (see (A.7)) is the joint probability density of random variables $x(\cdot, t)$ and $v(\cdot, t)$ or, equivalently, the probability density of random variable

$$\begin{pmatrix} x(\cdot, t) \\ v(\cdot, t) \end{pmatrix}, \quad t \geq t_0,$$

under the condition that $q_*(\xi, t) = Q$ (see (4.13) and (2.9)). Probability density $\mu_*(t, X, \cdot, U, Z)$ (see (A.3)) is the conditional probability density of the particle-velocity random variable $v(\cdot, t)$ under the conditions that the particle-position vector at time $t$ is equal to $X$, i.e., $x(\xi, t) = X$, and $q_*(\xi, t) = Q$. Probability density $\lambda_*(t, \cdot, U, Z)$ (see (A.5)) is the conditional probability density of the particle-position random variable $x(\cdot, t)$ under the condition that $q_*(\xi, t) = Q$.

REMARK A.1. Physically, concentration function $n_*(t, U, Z)$ is always uniformly bounded on $\Omega(t)$ for every fixed $t \geq t_0, U \in Y_*(t)$, and $Z \in Z_*(t)$. In particular, function $n_*(t, \cdot, U, Z)$ can never be the Dirac delta-function defined on $\mathbb{R}^3$. Thus, there are functions in space $L^1(\Omega(t))$ which cannot serve as $n_*(t, \cdot, U, Z)$. On the other hand, the physical reasoning assuring existence of real $k \in (1, \infty)$ such that $n_*(t, \cdot, U, Z) \in L^k(\Omega(t))$ is unclear. In other words, a proper function Banach space for the concentration function is still to be revealed.

The issues in Remark A.1 can help to better balance the formal and informal aspects in both theoretical and practical treatments of $n_*(t, \cdot, U, Z)$.

REFERENCES


