Fractional diffusant model of a multicomponent inhomogeneous gas mixture as a basis for the diffusant approximation

B M Burakhanov
Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13, Bldg 2, Moscow 125412, Russian Federation
E-mail: burbm@rambler.ru

Abstract. It can be shown that for a correct description of the motion of an inhomogeneous multicomponent mixture of gases, such concepts as a multi-velocity continuum and interpenetrating motion are not enough. This is the basis for the introduction of the concept of "poly-velocity motion". The reason for the need to use this concept is that to describe the motion of each component of an inhomogeneous mixture, it is necessary to use not one, but two velocity fields. The use of two velocity fields to describe the motion of a mixture component is the basis for constructing a fractional model of the mixture component, in which each component is divided into two fractions. This model serves as the basis for constructing the proposed fractional diffusant model of a multicomponent inhomogeneous gas mixture.

1. Introduction
The study of the behavior of multicomponent inhomogeneous gas-liquid mixtures is one of the main areas of research in hydrodynamics. The theories of these mixtures are based on the following concepts: multi-velocity continuum and interpenetrating motions [1], [2]. In addition, these theories postulate that for each component of the mixture, the equations of conservation of mass, momentum, and energy can be written.

Based on these theories, a hypothetical simplified model of a multicomponent inhomogeneous mixture, known as the diffusion approximation, is constructed [2].

The key concepts of the diffusion approximation are: barycentric velocity and diffusion velocity, and the main hypothesis of this approximation is the hypothesis that the density of the substance carried by diffusion flows can be assumed to be equal to the density of the considered component of the mixture.

In this paper, the inconsistency of this hypothesis is shown by a concrete example, from which the inconsistency of the diffusion approximation itself follows. The inadequacy of the diffusion approximation makes it relevant to search for alternative approximations. One of such alternative approximations is the diffusant approximation proposed in this paper.

The diffusant approximation is based on the fractional diffusant model of a component of an inhomogeneous multicomponent mixture proposed in [3]. In this fractional diffusant model, each i-th component $N_i$ of an inhomogeneous multicomponent mixture $N_0$ is divided into two fractions: the convective fraction $N_{vi}$ and the molecular relay fraction or diffusant $N_{wi}$. The main classification distinguishing feature of the diffusant $N_{wi}$ is: poly-velocity type of motion, which includes two
different mono-velocity types of motion. One of these types of motion is the
mono-velocity convective type of motion, which is motion together with the environment. The second
type of motion is the mono-velocity molecular relay race type of motion, which is a motion relative to
the environment. The main difference between the proposed diffusant approximation and the
traditional diffusion approximation is that the diffusant approximation is based on the concept of
"poly-velocity type of motion" and on the postulate that the magnitude of the modulus of the diffusant
velocity is one of the physical characteristics of an inhomogeneous multicomponent mixture.

2. Basic concepts and hypotheses of the diffusion approximation
The basic concepts of the mechanics of multi-velocity continua in general and the diffusion
approximation in particular are the concepts of multi-velocity continuum and interpenetrating motions
[2].
While the two main hypotheses of the diffusion approximation are:
- the hypothesis that the motion of each i-th \{i=1,...,n\} component \(N_i\) of a multicomponent
mixture \(N_0\) can be described by a single velocity field \(v_i\);
- the hypothesis that the value of the density \(\rho_i\) of the mass transferred by the diffusion fluxes of
the mass \(J_{i\alpha}\) can be assumed to be equal to the density of the component of the mixture \(N_i\).

When using the term – diffusion flow, it should be taken into account that in physics there are two
types of diffusion flows: the diffusion flow of the mass \(J_{i\alpha}\) and the concentration diffusion flow \(J_{\alpha\alpha}\). The relation that establishes the relationship between these two types of diffusion flows has the form

\[
J_{i\alpha} = \mu J_{\alpha\alpha}
\]  

(1)

where \(\mu\) is the mass of a single atom or molecule.
In addition, it should be taken into account that there are two main forms of diffusion fluxes of mass
\(J_{i\alpha}\): the physical form of recording, which has the form

\[
J_{i\alpha} = -D_i \nabla \rho_i
\]  

(2)

where \(D_i\) is the diffusion coefficient, and the hydrodynamic form of the record, which has the form

\[
J_{i\alpha} = \rho_{iJ} w_{Ji}
\]  

(3)

where \(\rho_{iJ}\) is the density of the mass diffusion flow, and \(w_{Ji}\) is its velocity.
From the validity of the expression (3) follows the validity of the expression of the form

\[
w_{Ji} = \frac{J_{i\alpha}}{\rho_{iJ}}.
\]  

(4)

One of the main postulates of the diffusion approximation is the postulate that the value of the
density \(\rho_{iJ}\) of the diffusion flow of mass \(J_{i\alpha}\) can be assumed to be equal to the value of the density \(\rho_i\)
of the component \(N_i\), that is, it is postulated that

\[
\rho_{iJ} = \rho_i
\]  

(5)

One of the key concepts of the diffusion approximation is the concept of the average - mass
velocity or barycentric velocity \(v_0\). The ratio that allows you to determine the value of this speed has the form

\[
v_0 = \sum_{i=1}^{n} \frac{\rho_i}{\rho_0},
\]  

(6)

where \(\rho_0 = \sum_{i=1}^{n} \rho_i\).
Another basic concept of this approximation is the concept - diffusional velocity \(w_i\), defined as
\[ w_i = v_i - v_0 \]  

(7)

It is easy to check that with such a determination of the diffusional velocity \( w_i \), the expression of the form

\[
\sum_{i=1}^{n} \rho_i w_i = 0
\]

(8)
is valid.

3. The basic system of equations of the diffusion approximation

When using the diffusion approximation, the continuity equation for the density \( \rho_i \) of the component \( N_i \) is written as [2]

\[
\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i v_i = \nabla \cdot (\rho_i w_i) + \sum_{j=1}^{m} J_{ij}
\]

(9)

where \( J_{ij} \) are the source terms that characterize the intensity of the transition of the mass from the component of the mixture \( N_i \) to the considered component of the mixture \( N_i \). Given the expressions (7) and (8), we obtain that the continuity equation for the mixture as a whole can be written as

\[
\frac{\partial \rho_0}{\partial t} + \nabla \cdot \rho_0 v_0 = 0
\]

(10)

It is shown in [2] that when using the diffusion approximation, the equation of motion describing the motion of the \( i \)–th component of the mixture has the form

\[
\frac{\partial \rho_i v_i}{\partial t} + \nabla \cdot \rho_i v_i v_0 = -\nabla \cdot \rho_i w_i w_i^k + \nabla \cdot \sigma_i^k + \rho_i g + \sum_{j=1}^{m} J_{ij}
\]

(11)

where \( \sigma_i = \sigma_i^k \) are the components of the surface force tensor, and \( g \) is the acceleration of gravity. Summing up the expressions (11) with respect to \( i \), we can obtain the equation of motion for the mixture as a whole, which has the form [2]

\[
\frac{\partial \rho_0 v_0}{\partial t} + \nabla \cdot \rho_0 v_0 v_0^k = -\sum_{i=1}^{n} \nabla \cdot \rho_i w_i w_i^k + \sum_{i=1}^{n} \nabla \cdot \sigma_i^k + \rho_0 g
\]

(12)

Neglecting the terms containing second-order quantities with respect to the diffusion velocities \( w_i^k \), we obtain

\[
\frac{\partial \rho_0 v_0}{\partial t} + \nabla \cdot \rho_0 v_0 v_0^k = \sum_{i=1}^{n} \nabla \cdot \sigma_i^k + \rho_0 g
\]

(13)

The energy equation for the \( i \)–th component of the mixture can be written as[2]

\[
\frac{\partial}{\partial t} \left( \rho_i \left( u_i + (|v_0|^2 + |w_i|^2)/2 \right) + \nabla \cdot (\rho_i (u_i + (|v_0|^2 + |w_i|^2)/2)) \right)v_i
\]

\[
= \nabla \cdot (\sigma_i^k v_i - q_i^k) + \rho_i g v_i + \sum_{j=1}^{m} E_{ij}
\]

(14)

where \( u_i \) is the internal energy of the \( i \)–th component of the mixture, and \( q_i^k \) is the components of the
vector that characterizes the external heat inflow, and \( E_{ij} \) describes the intensity of energy exchange between the components of the mixture.

The energy equation written for the mixture as a whole has the form [2]

\[
\frac{\partial}{\partial t} \left( \rho_i (u_i + |v_i|^2 / 2) + \sum_{k=1}^{n_i} \rho_k |w_k|^2 / 2 \right) + \nabla \cdot \left( \rho_i (u_i + |v_i|^2 / 2) + \sum_{k=1}^{n_i} \rho_k |w_k|^2 / 2 \right) v_i = - \nabla k (\sigma^k_i v_i - q^k_i) + \sum_{k=1}^{n_i} \rho_k g_i
\]

(15)

The complete system of equations of the diffusion approximation includes the equations (9), (10), (13) and (15) [2].

4. Diffusion and diffusant approaches to the construction of models of multicomponent inhomogeneous mixtures

It was noted above that there are physical and hydrodynamic forms of recording diffusion fluxes of mass \( J_{ni} \) and concentration diffusion fluxes \( J_{ni} \). Recall that the physical form of recording the density of concentration diffusion flows \( J_{ni} \), has the form

\[
J_{ni} = - D_i \nabla n_i
\]

(16)

where \( n_i \) is the density of the concentration diffusion flow \( J_{ni} \), and \( \nabla n_i \equiv |\nabla n_i| \hat{i} \) is here the guiding ort of the gradient vector \( \nabla n_i \), and the hydrodynamic form is written as

\[
J_{ni} = n_i w_i
\]

(17)

where \( w_i \) is the velocity of the concentration diffusion flow \( J_{ni} \). If we rewrite expression (17) in the form

\[
J_{ni} = n_i |w_i| \hat{i}_{ji}
\]

(18)

where \( \hat{i}_{ji} \) is the guiding ort of the concentration diffusion flow \( J_{ni} \), then it becomes obvious that to set the vector field \( J_{ni}(n_i, |w_i|, \hat{i}_i) \); it is necessary to set two scalar functions \( n_i \) and \( |w_i| \). In addition, it is necessary, using Fick’s law (16), to set the unit vector field \( \hat{i}_i \).

With the diffusion approach to the construction of models of inhomogeneous multicomponent mixtures, it is assumed that the density value \( n_{ij} \) of the same concentration diffusion flow \( J_{ni} \) is equal to the concentration value \( n_{ni} \) of the component of the mixture \( N_i \).

With the diffusant approach to constructing models of inhomogeneous multicomponent mixtures, it is assumed that the magnitude of the modulus \( |w_{ji}| \) velocity \( w_{ji} \) of the concentration diffusion flow \( J_{ni} \) is equal to the value of the average velocity of the thermal motion of the molecules \( v_{ti} \) of the component of the mixture \( N_i \).

From a physical point of view, the postulate that the values of the modulus \( |w_{ji}| \) velocity \( w_{ji} \) are equal to the value of the average velocity of thermal motion of molecules \( v_{ti} \) is equivalent to the postulate that the magnitude of the velocity modulus of diffusion flows \( J_{ni} \) belongs to the main thermodynamic characteristics of a multicomponent inhomogeneous mixture.

It is obvious that in order to establish the fact that the magnitude of the modulus \( |w_{ji}| \) velocity \( w_{ji} \) of the concentration diffusion flow \( J_{ni} \) belongs to the main thermodynamic characteristics of multicomponent inhomogeneous mixtures, it is sufficient to establish this fact for any particular mixture.

One of such particular mixtures is considered in [3] and is a stationary inhomogeneous mixture of...
two isotopes $C_{i,1}$ and $C_{i,2}$ of an ideal gas $C$, located at constant temperature and pressure. In this work, it is shown that the values of the velocity modulus function of the diffusion fluxes contained in this stationary mixture should be considered equal to the values of the function of the average velocity of the thermal motion of the molecules of the isotopes $C_{i,1}$ and $C_{i,2}$.

5. Proof of the failure of the main hypothesis of the diffusion approximation
In this case, the main hypothesis of the diffusion approximation is understood to be the postulate that the concentration value $n_i$ of molecules forming concentration diffusion flows $J_{ni}$ can be assumed to be equal to the concentration value $n_{Ni}$ of molecules forming the component $N_i$ of a multicomponent inhomogeneous mixture $N_i$.

It follows from the results of [3] that the use of this hypothesis in analyzing the behavior of a stationary inhomogeneous mixture of two isotopes $C_{i,1}$ and $C_{i,2}$ of an ideal gas C, located at constant temperature and pressure, leads to a violation of the law of conservation of energy.

Recall that in the thought experiment discussed in [3], an inhomogeneous mixture of isotopes $C_{i,1}$ and $C_{i,2}$ of an ideal gas placed in a rectangular parallelepiped, at the boundaries of which stationary boundary conditions are set, such that along the axis of this parallelepiped there should be a linear distribution of concentrations of $n_{C1}$ and $n_{C2}$ molecules of isotopes $C_{i,1}$ and $C_{i,2}$. As a result of the existence of this stationary linear distribution of the concentrations $n_{C1}$ and $n_{C2}$ in the parallelepiped, there should be two equal in modulus and opposite in direction stationary concentration diffusion flows $J_{C1}$ and $J_{C2}$.

From the stationarity of the thought experiment considered in [3], it follows that the amount of substance and the amounts of momentum and the amount of kinetic energy of each isotope that enter and leave this parallelepiped through its end side surfaces must be equal to each other. In other words, in this experiment, a mixture of isotopes $C_{i,1}$ and $C_{i,2}$ placed in a parallelepiped acts no more than as an intermediary providing the exchange of matter and momentum and energy between external objects located to the left and right of the end surfaces of the parallelepiped.

It turns out that the absence of an exchange of matter and momentum and energy between external objects and a mixture of isotopes $C_{i,1}$ and $C_{i,2}$ located in a parallelepiped is possible only if the magnitude of the modulus $|w|$ velocity $w$ of the oncoming diffusion fluxes $J_{C1}$ and $J_{C2}$ existing in the parallelepiped is constant and equal to the value of the average velocity of thermal motion of molecules of isotopes $C_{i,1}$ and $C_{i,2}$.

From the above-mentioned basic hypothesis of the diffusion approximation, it follows that in the case of a linear decrease in the concentrations of $n_{C1}$ and $n_{C2}$ isotopes of $C_{i,1}$ and $C_{i,2}$ along the axis of the parallelepiped, the velocity of the oncoming diffusion fluxes $J_{C1}$ and $J_{C2}$ should simultaneously increase. In addition, with an increase in the velocity of diffusion flows, the amount of kinetic energy transferred by these flows should simultaneously increase. As a result, the amount of kinetic energy leaving the parallelepiped must exceed the amount of kinetic energy entering this parallelepiped. This means that this parallelepiped is an infinitely capacious source of kinetic energy.

This circumstance indicates the inadmissibility of using the basic hypothesis of the diffusion approximation in the study of the behavior of multicomponent inhomogeneous mixtures. Moreover, the failure of the main hypothesis of the diffusion approximation implies the failure of the diffusion approximation itself.

6. Fractional diffusant model of a component of a multicomponent inhomogeneous mixture
In [3], a fractional diffusant model of a component of a multicomponent inhomogeneous mixture was proposed. This model is based on the postulate that each component $N_i$ of an inhomogeneous multicomponent mixture $N_i$ consists of two fractions: the convective fraction $N_{wi}$ and the diffusant fraction or simply diffusant $N_{wi}$.

In this case, the basis for dividing the component of the mixture $N_i$ into the convective fraction $N_{wi}$ and the diffusant $N_{wi}$ is the presence of three classification distinguishing features in the diffusant $N_{wi}$,
Two distinctive physical features of the diffusant are:
- poly-velocity type of diffusant motion, including portable motion described by the field of portable diffusant velocities \( \mathbf{w}_0 \), coinciding with the field of convective velocities \( \mathbf{v}_0 \) of the mixture as a whole, and relative motion described by the field of relative diffusant velocities \( \mathbf{w}_J \);
- belonging of the modules \( |\mathbf{w}_{ni}| \) of the field of relative diffusion velocities \( \mathbf{w}_J \) to the number of thermodynamic characteristics of a multicomponent inhomogeneous mixture.

While one distinctive mathematical feature of a diffusant is that the field of relative diffusant velocities \( \mathbf{w}_J \) belongs to the number of layered vector fields [5].

The presence of any of these three distinctive features is sufficient for a reasonable introduction to the consideration of "diffusant \( N_{wi} \)". It makes sense to consider the concept of "diffusant" introduced in this way as a generalized concept that includes various particular types of this concept.

These particular types of the generalized concept of "diffusant \( N_{wi} \)" include:
- "particle quantity diffusant" or " concentration diffusant \( N_{wmi} \)" consisting of the number of molecules of the type under consideration associated with particles of concentration diffusion flows \( \mathbf{J}_{ni} \);
- " mass diffusant \( N_{wmi} \) " associated with the amount of substance carried by particles forming concentration diffusion flows \( \mathbf{J}_{ni} \);
- "pulse diffusant \( N_{wp} \) " associated with the amount of motion carried by particles forming concentration diffusion flows \( \mathbf{J}_{ni} \);
- "energy diffusant \( N_{wEi} \) " associated with the amount of kinetic energy transferred by particles forming concentric diffusion flows \( \mathbf{J}_{ni} \).

It is essential that all the above-mentioned particular types of diffusants have the property of conservation.

7. Mono-velocity and poly-velocity types of multi-velocity continuum

It was mentioned above that in hydrodynamics, the construction of models of multicomponent inhomogeneous mixtures is based on the concepts of "multi-velocity continuum" and "interpenetrating motions". In addition, it was mentioned above that one of the main hypotheses currently used in the mechanics of inhomogeneous mixtures is the hypothesis that the motion of each component \( N_i \) of a multicomponent mixture \( N_0 \) can be described by a mono-velocity field \( \mathbf{v}_i \).

Considering that, by definition, a mono-velocity type of motion is a motion that can be described by a mono-velocity field, it is possible to introduce the concept of a "mono-velocity type of a multi-velocity continuum" into consideration. By definition, a mono-velocity type of poly-velocity continuum is a multi-velocity continuum, which is a superposition of mono-velocity continua. It follows from this definition that continua that are currently used in hydrodynamics in constructing models of multicomponent inhomogeneous mixtures belong to this type of multi-velocity continua.

When constructing fractional models of multicomponent inhomogeneous mixtures \( N_0 \) based on fractional models of the component \( N_i \) of the mixture \( N_0 \), it is necessary to take into account that the motion of the component \( N_i \) of the mixture \( N_0 \) belongs to a poly-velocity type of motion, for the description of which it is necessary to use two velocity fields: the portable diffusant velocity field \( \mathbf{w}_0 = \mathbf{v}_0 \) and the relative diffusant velocity field \( \mathbf{w}_J \).

It is assumed that, by definition, a poly-velocity type of a multi-velocity continuum is called a continuum, which is a superposition of continua, to describe the movement of some parts of which it is necessary to use several velocity fields. From this definition it follows that it is to this type of multi-velocity continua that continua belong, which must be used in hydrodynamics when constructing fractional models of multicomponent inhomogeneous mixtures.

8. The basic system of diffusant approximation equations

Using Fick's law, it is easy to find the ort \( i_s = (\mathbf{J}_s / |\mathbf{J}_s|) \) of the density vector of the diffusion mass flow \( \mathbf{J}_s \). In addition, postulating that the magnitude of the modulus \( |\mathbf{w}_J| \) of the diffusant velocities \( \mathbf{w}_J \)
can be considered equal to the value of the average velocity of the thermal motion of atoms and molecules $v_T$, it is easy to obtain expressions of the form

$$J_{pi} = \rho_{ji} v_{ni} i_{pi}$$  \hspace{1cm} (19)

$$\rho_{ji} = |J_{pi}| / v_{ni}$$  \hspace{1cm} (20)

Knowing the value of the diffusant density $\rho_{ji}$, it is easy to find the value of the density $\rho_{vi}$ of the convective fraction $N_v$. To do this, it is enough to use an expression of the form

$$\rho_{ji} + \rho_{vi} = \rho_i.$$  \hspace{1cm} (21)

When using the diffusant approximation, the continuity equation written for the density value $\rho_i$ of the component $N_i$ has the form

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i \mathbf{v} = -\nabla \cdot \rho_i \mathbf{v} \rho_{ji} + \sum_{j=1}^{m} J_{ij},$$  \hspace{1cm} (22)

where $J_{ij}$ are the source terms that characterize the intensity of the transition of the substance from the component of the mixture $N_j$ to the considered component of the mixture $N_i$. Summing these equations with respect to $i$, we obtain the continuity equation for the mixture $N_0$ as a whole, which has the form

$$\frac{\partial \rho_0}{\partial t} + \nabla \cdot \rho_0 \mathbf{v} = 0$$  \hspace{1cm} (23)

In the diffusant approximation, the equation of motion describing the motion of the component $N_i$ has the form

$$\frac{\partial \rho_i \mathbf{v}}{\partial t} + \nabla \cdot \rho_i \mathbf{v} \mathbf{v}^k = -\nabla \cdot \rho_i \mathbf{v} \rho_{ji} \mathbf{w}_{ji}^k + \nabla \cdot \rho_i \mathbf{v} \sigma_i^k + \rho_i \mathbf{g} + \sum_{j=1}^{m} P_{ij}$$  \hspace{1cm} (24)

Summing up equations (24) with respect to $i$, we obtain

$$\sum_{i=1}^{n} \frac{\partial \rho_i \mathbf{v} \mathbf{v}^k}{\partial t} + \nabla \cdot \rho_0 \mathbf{v} \mathbf{v}^k = \sum_{i=1}^{n} \nabla \cdot \rho_i \mathbf{v} \mathbf{v}^k + \sum_{i=1}^{n} \nabla \cdot \rho_i \mathbf{v} \sigma_i^k + \rho_0 \mathbf{g}$$  \hspace{1cm} (25)

With the diffusant approximation, the energy equation written for the $i$-th component $N_i$ of the mixture $N_0$ can be represented as

$$\frac{\partial}{\partial t} \left( \rho_i (u_i + |\mathbf{v}|^2 / 2 + \rho_{ji} v_{ni}^2 / 2) \right) + \nabla \cdot \left( \rho_i (u_i + |\mathbf{v}|^2 / 2 + \rho_{ji} v_{ni}^2 / 2) \mathbf{v}^k \right)$$

$$= -\nabla \cdot \left( \rho_i (u_i + |\mathbf{v}|^2 / 2 + \rho_{ji} v_{ni}^2 / 2) \mathbf{w}_{ji}^k \right) + \nabla \cdot \left( \rho_i (u_i + |\mathbf{v}|^2 / 2 + \rho_{ji} v_{ni}^2 / 2) \mathbf{q}_i^k \right) + \rho_i \mathbf{g} \mathbf{v} + \rho_i \mathbf{g} \mathbf{w}_{ji} + \sum_{j=1}^{m} E_{ij}$$  \hspace{1cm} (26)

Summing up equations (26) with respect to $i$, we obtain

$$\sum_{i=1}^{n} \frac{\partial}{\partial t} \left( \rho_i (u_i + |\mathbf{v}|^2 / 2 + \rho_{ji} v_{ni}^2 / 2) \right) + \sum_{i=1}^{n} \nabla \cdot \left( \rho_i (u_i + |\mathbf{v}|^2 / 2 + \rho_{ji} v_{ni}^2 / 2) \mathbf{v}^k \right)$$

$$= -\nabla \cdot \left( \rho_0 (u_i + |\mathbf{v}|^2 / 2 + \rho_{ji} v_{ni}^2 / 2) \mathbf{w}_{ji}^k \right) + \nabla \cdot \left( \rho_0 (u_i + |\mathbf{v}|^2 / 2 + \rho_{ji} v_{ni}^2 / 2) \mathbf{q}_i^k \right) + \rho_0 \mathbf{g} \mathbf{v} + \rho_0 \mathbf{g} \mathbf{w}_{ji} + \sum_{j=1}^{m} E_{ij}$$  \hspace{1cm} (27)
The complete system of equations of the diffusant approximation includes the equations (22), (23), (25) and (27).

9. Conclusions
The main results of this work are:
1. Examples are given that prove the inconsistency of the diffusion approximation.
2. A fractional diffusant model of the mixture component is described.
3. Classification distinguishing features of fractions forming components of multicomponent mixtures are established.
4. A diffusant approximation is proposed.

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