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A Comparative Study of Non-Fickean Diffusion in Binary Fluids

by
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Abstract

We consider a non-Fickean diffusion model for binary mixtures. Here, the flux is not governed by Fick's law, it is governed by an evolution equation, derived from the partial balance momenta under the hypothesis of "small" diffusion velocities. We apply this model to a binary non-reactive mixture with zero average velocity at thermal equilibrium. In particular, Fick's model is recovered as a first order perturbation of the non-Fickean model.

Key words and phrases: *diffusion models, hyperbolic PDE, parabolic PDE, asymptotic limit.*

1 Introduction

Fick law constitutes the most used model of diffusion processes in fluid mixtures. In this approach the time evolution of the concentration of the constituents is governed by a parabolic partial differential equation. A major drawback of the model is given by that in the context of linearized theory it predicts infinite speed propagation of the perturbation. This fact is known as the paradox of the diffusion theory.

This paradox can be excluded by considering an evolution equation for the diffusive flux instead of Fick law [1]. The new equation results from the equation of partial momenta and the equation of global momentum. In the sequel, we briefly describe how one can obtain this equation. For more general informations in the theory of the mixtures, the reader is referred to [1],[2].

The mixture can be considered as a single fluid if one thinks that each position $\boldsymbol{x}$ may be occupied simultaneously by several different particles $\boldsymbol{X}_a$, one for each constituent a. Each constituent has its individual density ρ_a and its individual velocity $\boldsymbol{v}_a$, $a = 1, ..., n$. The mass density ρ and the velocity $\boldsymbol{v}$ of the mixture are defined by

$$\rho = \sum \rho_a, \ \ \boldsymbol{v} = \sum \frac{\rho_a}{\rho} \boldsymbol{v}_a. \tag{1}$$

Assuming that there exists a unique temperature T for all constituents, the fields $\rho_a(\boldsymbol{x}, t)$, $\boldsymbol{v}_a(\boldsymbol{x}, t)$, $T(\boldsymbol{x}, t)$, for all $a = 1, ..., n$ are determined by solving the equations of mass balance, momentum balance

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of the constituents and the equation of balance for energy of the mixture. In the absence of the external forces and external radiation sources, these balance laws read

$$\begin{aligned} \partial_t\rho_a + \partial_i\rho_a v_a^i &= \widetilde{m}_a, \\ \partial_t\rho_a v_a^j + \partial_i(\rho_a v_a^i v_a^j - t_a^{ji}) &= \widetilde{h}_a^j, \\ \partial_t\rho(\varepsilon + 1/2v^2) + \partial_i(\rho(\varepsilon + 1/2v^2)v^i - t^{ij}v_j + q^i) &= 0, \end{aligned} \tag{2}$$

where $\widetilde{m}_a$ represents internal mass production due to the chemical reactions, $\widetilde{h}_a$ represents the internal production of partial momentum due to the collisions between different constituents and $\boldsymbol{t}_a$ denotes the partial stress tensor. In the last equation resulting from the balance of total energy $\varepsilon, \boldsymbol{t}, \boldsymbol{q}$ stand for internal energy, stress tensor and heat of the mixture, respectively.
By summing up the mass and momentum equations one obtain the continuity equation and the momentum equations for the mixture

$$\begin{aligned} \partial_t\rho + \partial_i\rho v^i &= 0 \\ \partial_t\rho v^j + \partial_i(\rho v^i v^j - t^{ij}) &= 0 \end{aligned} \tag{3}$$

One defines the diffusion velocity of the first constituent, as $\boldsymbol{u} = \boldsymbol{v}_1 - \boldsymbol{v}$, its diffusion flux as $\boldsymbol{J} = \rho_1\boldsymbol{u}$ and its mass concentration by $c = \dfrac{\rho_a}{\rho}$. We consider, $c(\boldsymbol{x}, t)$, $\boldsymbol{J}(\boldsymbol{x}, t)$, $\rho(\boldsymbol{x}, t)$, $\boldsymbol{v}(\boldsymbol{x}, t)$, $T(\boldsymbol{x}, t)$ as state variables for the binary fluid.
The equation (2_1) can be rewritten as

$$\partial_t\rho c + \partial_i(\rho c v^i + J^i) = \widetilde{m}. \tag{4}$$

This equation and the Fick law

$$\boldsymbol{J} = -\rho D\nabla c, \tag{5}$$

constitute the classical kinetic model of diffusion processes, i.e the Fickean model.
A non-Fickean model for diffusion processes can be defined as a model in which Fick's law is no longer true. Here, we develop a non-Fickean model. We have the following identities

$$\rho_1\boldsymbol{v}_1 = \boldsymbol{J} + c\rho\boldsymbol{v}, \quad \rho_1 v_1^i v_1^j = J^i v^j + J^j v^i + c\rho v^i v^j + \rho_1(v_1^i - v^i)(v_1^j - v^j).$$

By neglecting the quadratic term in diffusion velocity, we approximate the equation (2_2) by

$$\partial_t\left(\boldsymbol{J} + c\rho\boldsymbol{v}\right) + \nabla\cdot(\boldsymbol{J}\otimes\boldsymbol{v} + \boldsymbol{v}\otimes\boldsymbol{J} + c\rho\boldsymbol{v}\otimes\boldsymbol{v} - \boldsymbol{t}_1) = \widetilde{\boldsymbol{h}}. \tag{6}$$

Using (3) and (4), the equation (6) can be written as

$$\partial_t\boldsymbol{J} + \nabla\cdot(\boldsymbol{J}\otimes\boldsymbol{v} + \boldsymbol{v}\otimes\boldsymbol{J}) - \boldsymbol{v}\nabla\cdot\boldsymbol{J} + c\nabla\cdot\boldsymbol{t} - \nabla\cdot\boldsymbol{t}_1 = \widetilde{\boldsymbol{h}} - \boldsymbol{v}\widetilde{m} \tag{7}$$

As in [1], we assume that the production of partial momentum $\widetilde{\boldsymbol{h}}$ has the form

$$\widetilde{\boldsymbol{h}} = \boldsymbol{v}_1\widetilde{m} + M^{11}\frac{\rho}{\rho_1\rho_2}\boldsymbol{J}. \tag{8}$$

Concerning the constitutive relations for the stress tensor, we assume that each constituent of the mixture, as well as the mixture are inviscide fluids. Then, the constitutive relations for the stress tensor are given by

$$t_a^{ij} = -p_a \delta^{ij}, \quad t^{ij} = -p\delta^{ij}, \tag{9}$$

where p_a and p represent the partial pressure and total pressure, respectively. Another constitutive assumption is the *Dalton law*

$$p_a = c_a p \tag{10}$$

The assumptions (8), (9) and (10) lead to

$$\partial_t \boldsymbol{J} + \nabla \cdot (\boldsymbol{J} \otimes \boldsymbol{v} + \boldsymbol{v} \otimes \boldsymbol{J}) - \boldsymbol{v} \nabla \cdot \boldsymbol{J} + p \nabla c = \left(\frac{\widetilde{m}}{\rho_1} + M^{11} \frac{\rho}{\rho_1 \rho_2} \right) \boldsymbol{J}. \tag{11}$$

We conclude that the basic equations describing the non-Fickean diffusion for binary inviscide reactive mixture are: the equation of balance for the total energy (2_3), the equations of balance for mass and momentum (3) with the stress tensor given by (9), the equation of the partial mass production (4) and the equation for partial momenta (11). Besides these equations, one must add constitutive laws regarding the internal energy $\varepsilon(\rho, T)$, the state equation $p(\rho, T)$, the mass production $\widetilde{m}(c, \rho, T)$ and for the coefficient $M^{11}(c, \rho, T)$ appearing in the partial momenta production.

2 Telegraph Equation as Model for Non-Fickean Diffusion

In this section we analyse a simplified case of non-Fickean diffusion. We consider a non-reactive mixture at rest, at thermal equilibrium. Then the temperature $T(t, \boldsymbol{x})$ and the mass density $\rho(t, \boldsymbol{x})$ are constant fields, (say $T_0, \rho_0,$) and the velocity $\boldsymbol{v}$ is a null field.
The only variable fields considered here are the concentration $c(t, x)$ and its diffusion flux $J(t, x)$ depending on the time $t > 0$ and the position $x \in \mathbb{R}$. The governing equation are given by

$$\begin{aligned} \rho_0 \partial_t c + \partial_x J &= 0, \\ \partial_t J + p_0 \partial_x c &= M^{11} \frac{\rho_0}{\rho_1 \rho_2} J. \end{aligned}$$

Assume that the coefficient M^{11} has the following dependence on ρ_1 and ρ_2

$$M^{11} \frac{\rho_0}{\rho_1 \rho_2} = -\frac{p_0}{\rho_0 D}. \tag{12}$$

We obtain

$$\begin{aligned} \rho_0 \partial_t c + \partial_x J &= 0, \\ \frac{\rho_0 D}{p_0} \partial_t J + \rho_0 D \partial_x c &= -J. \end{aligned} \tag{13}$$

Note that, if the first term on the l.h.s of the second equation is dropped out, one obtain the Fick law for diffusion. Our purpose is *to compare the solution given by equations* (14) *with the solution of classical diffusion equation.*

It is more convenient to work with dimensionless variable. As we can see, the explicit parameters in equations (14) are p_0, ρ_0 and D. We are interested in defining a characteristic time and a characteristic length. For our purpose, it not proper to use the characteristic length as a combinations of p_0, ρ_0 and D.
Let L be a characteristic length. Consider D to be another characteristic dimension of the problem. We introduce the following dimensionless quantities:

$$t = L^2 D^{-1}\widetilde{t}, x = L\widetilde{x}, J = \rho_0 D L^{-1}\widetilde{J}.$$

The dimensionless form of equations (14) can be written

$$\begin{aligned} \partial_t c + \partial_x J &= 0, \\ \varepsilon \partial_t J + \partial_x c &= -J, \end{aligned} \tag{14}$$

where the dimensionless parameter ε is given by

$$\varepsilon = \frac{D^2}{L^2}\frac{\rho_0}{p_0}. \tag{15}$$

If one eliminates the diffusive flux from the equations (14), one obtains equation for the mass concentration. This equation is known as the telegraph equation

$$\varepsilon \partial_t^2 c + \partial_t c = \partial_x^2 c. \tag{16}$$

We point out two important facts related to the non-Fickean model introduced above:
(a) The time evolution of mass concentration is governed by a hyperbolic equation, instead of parabolic equation as in Fick's model,
(b) The Fick model can be viewed as first order perturbation of the present model.
We consider the Cauchy problem for (14) with the initial conditions:

$$\big(c, J\big)\big|_{t=0} = \big(c_0(x), J_0(x)\big). \tag{17}$$

Let

$$\boldsymbol{u} = \begin{pmatrix} c \\ J \end{pmatrix}, \quad \boldsymbol{A}_\varepsilon = \begin{pmatrix} 0 & -\partial_x \\ -\varepsilon^{-1}\partial_x & -\varepsilon^{-1} \end{pmatrix}.$$

The Cauchy problem for the non-Fickean diffusion problem (NFDP) takes the form

$$\left\{ \begin{array}{l} \dfrac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \boldsymbol{A}_\varepsilon \boldsymbol{u} \\ \\ \boldsymbol{u}|_{t=0} = \boldsymbol{u}_0 \end{array} \right. . \tag{18}$$

We also consider the Cauchy problem for Fickean diffusion

$$\left\{ \begin{array}{l} \dfrac{\mathrm{d}w}{\mathrm{d}t} = \triangle w \\ \\ w|_{t=0} = c_0 \end{array} \right. . \tag{19}$$

Our main result is:

Theorem 2.1 *Assume that the initial datum* $\boldsymbol{u}_0$ *is a bounded continuous function and* u, $\partial_x u$, $\partial_x^2 u$ *belong to* $\mathbb{L}^2(\mathbb{R})$. *Let* $\boldsymbol{u}_\varepsilon(t,x)$ *be the the solution of the (NFDP),* $w(t,x)$ *be the solution of the (FDP). Then we have the following properties:*
(1) Finite speed of propagation. *If the initial datum* c_0 *has compact support, then the solution* $c_\varepsilon(t,x)$ *has also compact support for any finite time* t
(2) Fickean diffusion as singular asymptotic limit of non-Fickean diffusion. *The following relations hold*

$$\lim_{\varepsilon\to 0} c_\varepsilon(t,x) = w(t,x), \tag{20}$$

$$\lim_{\varepsilon\to 0} \left(J_\varepsilon(t,x) + \partial_x c_\varepsilon(t,x)\right) = 0. \tag{21}$$

Proof. The solution of the (NFDP) is obtained by using the Fourier transform. For any absolute integrable function ψ its Fourier transform is given by

$$\widetilde{\psi}(\xi) = \int_{\mathbb{R}^n} \exp(-\mathrm{i}x\cdot\xi)\psi(x)\mathrm{d}x.$$

The original problem for Fourier transform reads

$$\begin{cases} \dfrac{\mathrm{d}\widetilde{\boldsymbol{u}}}{\mathrm{d}t} = \boldsymbol{A}_\varepsilon(\xi)\widetilde{\boldsymbol{u}} \\ \\ \widetilde{\boldsymbol{u}}|_{t=0} = \widetilde{\boldsymbol{u}}_0(\xi) \end{cases} \tag{22}$$

where the matrix $\boldsymbol{A}_\varepsilon(\xi)$ has the expression

$$\boldsymbol{A}_\varepsilon = \begin{pmatrix} 0 & -\mathrm{i}\xi \\ -\varepsilon^{-1}\mathrm{i}\xi & -\varepsilon^{-1} \end{pmatrix}.$$

The Fourier transform of the solution is given by

$$\widetilde{\boldsymbol{u}}(t,\xi) = \widetilde{\boldsymbol{\mathcal{E}}}(t,\xi;\varepsilon)\widetilde{\boldsymbol{u}}_0(\xi).$$

Returning to the original variables, we have

$$\boldsymbol{u}(t,x) = \boldsymbol{\mathcal{E}}(t;\varepsilon) * \boldsymbol{u}_0(x). \tag{23}$$

By standard calculations, we obtain

$$\widetilde{\boldsymbol{\mathcal{E}}}(t,\xi;\varepsilon) := \mathrm{e}^{t\,\boldsymbol{A}_\varepsilon(\xi)} = \mathrm{e}^{-\dfrac{t}{2\varepsilon}} \begin{pmatrix} \omega_\varepsilon(t,\xi) + 2\varepsilon\partial_t\omega_\varepsilon(t,\xi) & -2\varepsilon\mathrm{i}\xi\omega_\varepsilon(t,\xi) \\ \\ -2\mathrm{i}\xi\omega_\varepsilon(t,\xi) & -\omega_\varepsilon(t,\xi) + 2\varepsilon\partial_t\omega_\varepsilon(t,\xi) \end{pmatrix},$$

where

$$\delta = \sqrt{1-4\varepsilon\xi^2}, \quad \omega_\varepsilon(t,\xi) = \frac{\mathrm{e}^{\dfrac{t\delta}{2\varepsilon}} - \mathrm{e}^{-\dfrac{t\delta}{2\varepsilon}}}{2\delta}.$$

(1) To demonstrate that the solution $c_\varepsilon(t,x)$ has compact support we calculate the convolution (23). The inverse Fourier transform of $\omega_\varepsilon(t,\xi)\widetilde{c}_o(\xi)$ is given by [3]

$$\phi_\varepsilon(t,x;c_0) = \frac{1}{4\sqrt{\varepsilon}} \int_{x-t/\sqrt{\varepsilon}}^{x+t/\sqrt{\varepsilon}} I\left(\frac{1}{2\varepsilon}\sqrt{t^2-\varepsilon(y-x)^2}\right) c_0(y)\mathrm{d}y,$$

where

$$I(z) = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} \mathrm{e}^{z\sin\phi}\mathrm{d}\phi.$$

Using this formula, we obtain

$$\begin{aligned}
\mathrm{e}^{t/2\varepsilon} c_\varepsilon(t,x) = \quad & \frac{c_0(x+t/\sqrt{\varepsilon}) + c_0(x-t/\sqrt{\varepsilon})}{2} + \\
& \frac{t}{4\varepsilon}\int_{-1}^{1}\left[I\left(t\frac{\sqrt{1-y^2}}{2\varepsilon}\right) + \frac{1}{\sqrt{1-y^2}} I'\left(t\frac{\sqrt{1-y^2}}{2\varepsilon}\right)\right] c_0(x+\frac{yt}{\sqrt{\varepsilon}})\mathrm{d}y \\
& -\sqrt{\varepsilon}\frac{j_0(x+t/\sqrt{\varepsilon}) - j_0(x-t/\sqrt{\varepsilon})}{2} - \\
& \frac{t}{4\varepsilon}\int_{-1}^{1}\frac{y}{\sqrt{1-y^2}} I'\left(t\frac{\sqrt{1-y^2}}{2\varepsilon}\right) j_0(x+\frac{yt}{\sqrt{\varepsilon}})\mathrm{d}y
\end{aligned}$$

and similarly for $j(t,x)$. From here, one obtains that if the initial data has compact support, then for any finite time the solution has also compact support.
(2) We have

$$\lim_{\varepsilon\to 0} \widetilde{\boldsymbol{\mathcal{E}}}(t,\xi;\varepsilon) = \begin{pmatrix} \mathrm{e}^{-\xi^2 t} & 0 \\ -\mathrm{i}\xi\mathrm{e}^{-\xi^2 t} & 0 \end{pmatrix}.$$

Observe that the function

$$\widetilde{w}(t,\xi) = \mathrm{e}^{-\xi^2 t}\widetilde{c}_0(\xi)$$

solves the (FDP). Taking into account that the elements $\widetilde{\boldsymbol{\mathcal{E}}}(t,\xi;\varepsilon)\widetilde{\boldsymbol{u}}_0$ are bounded by some square integrable functions, we obtain the first limit (20) ($L^2(\mathbb{R})$ convergence). The second limit in (21) is similarly proved.

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