ARTICLE IN PRESS

Nonlinear Analysis ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Nonlinear Analysis

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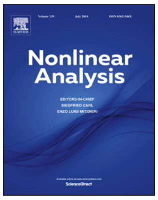

Maxwell–Stefan diffusion asymptotics for gas mixtures in non-isothermal setting

Harsha Hutridurga[a], Francesco Salvarani[b,c,*]

[a] *Department of Mathematics, Imperial College London, London, SW7 2AZ, United Kingdom*
[b] *Université Paris-Dauphine, Ceremade, UMR CNRS 7534, F-75775 Paris Cedex 16, France*
[c] *Università degli Studi di Pavia, Dipartimento di Matematica, I-27100 Pavia, Italy*

ARTICLE INFO

Article history:
Received 24 September 2016
Accepted 28 March 2017
Communicated by S. Carl

Keywords:
Maxwell–Stefan system
Boltzmann equation
Binary diffusion coefficients

ABSTRACT

A mathematical model is proposed where the classical Maxwell–Stefan diffusion model for gas mixtures is coupled to an advection-type equation for the temperature of the physical system. This coupled system is derived from first principles in the sense that the starting point of our analysis is a system of Boltzmann equations for gaseous mixtures. We perform an asymptotic analysis on the Boltzmann model under diffuse scaling to arrive at the proposed coupled system.

1. Introduction

The Maxwell–Stefan theory [23,27] has been the most successful approach for describing diffusive phenomena in gaseous mixtures, and it is now the reference model for studying multicomponent diffusion. The Maxwell–Stefan system is a coupled system of cross-diffusion equations and it is commonly used in many scientific fields, for e.g., in engineering [22] and in medical sciences [7,28].

Despite its current utility, the mathematical studies on the subject are however quite recent (see [17,15,16,18]). In particular, existence and uniqueness issues, as well as the long-time behaviour, have been considered in [6,10,21,13], whereas [24] deals with the numerical study of the Maxwell–Stefan equations.

In [11], the authors provide the formal derivation of the Maxwell–Stefan diffusion equations starting from the non-reactive elastic Boltzmann system for monatomic gaseous mixtures [12,14,9]. They show that the zeroth and first order moments of appropriate solutions of the Boltzmann system, in the diffusive scaling and for vanishing Mach and Knudsen numbers limit, formally converge to the solution of the Maxwell–Stefan equations. This result, which lies in the research line introduced by Bardos, Golse and Levermore in [1–3],

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[*] Corresponding author at: Università degli Studi di Pavia, Dipartimento di Matematica, I-27100 Pavia, Italy.
E-mail addresses: h.hutridurga-ramaiah@imperial.ac.uk (H. Hutridurga), francesco.salvarani@unipv.it (F. Salvarani).

http://dx.doi.org/10.1016/j.na.2017.03.019

Please cite this article in press as: H. Hutridurga, F. Salvarani, Maxwell–Stefan diffusion asymptotics for gas mixtures in non-isothermal setting, Nonlinear Analysis (2017), http://dx.doi.org/10.1016/j.na.2017.03.019

has been obtained in the framework of Maxwellian cross sections. Subsequently, the approach of [11] has been generalized in [8], where the Maxwell–Stefan diffusion coefficients have been written in terms of explicit formulas with respect to the cross-sections, and in [20] where the explicit dependence of the Maxwell–Stefan binary diffusion coefficients with respect to the temperature of the mixture has been obtained for general analytical cross sections satisfying Grad's cutoff assumption [19].

All the previous results have been obtained in the isothermal case. However, as pointed out by Krishna and Wesselingh, "perfectly isothermal systems are rare in chemical engineering practice and many processes such as distillation, absorption, condensation, evaporation and drying involve the simultaneous transfer of mass and energy across phase interfaces" [22, p.876].

For this reason, it is natural to extend the strategy of [11] to the non-isothermal case, and this is the purpose of the present article: we provide here the asymptotics of the Boltzmann system for monatomic mixtures that leads to a non-isothermal form of the Maxwell–Stefan equations, and thus we can take into account the thermal diffusion contribution to the molar fluxes (thermophoresis). We postulate that the solution of the Boltzmann system keeps the structure of a local Maxwellian and then we deduce, in the standard diffusive limit, the coupled relationships satisfied by the densities, the fluxes and the temperature at the macroscopic level which guarantee that the local Maxwellian structure is preserved by the time evolution of the system.

A major question is posed by the closure relationship. Indeed, as in the case of the Maxwell–Stefan system, the resulting equations for the densities, the fluxes and the temperature are, in the diffusive limit, linearly dependent and an additional equation between the unknowns is necessary in order to close it. As it is well known, in the isothermal Maxwell–Stefan system, the closure relationship consists in supposing that the sum of all molar fluxes J_i is locally identically zero. This supplementary equation could be incompatible with some experimental behaviours in the non-isothermal setting: as pointed out in [22], indeed, in chemical vapour deposition (CVD) processes, thermal diffusion causes large, heavy gas molecules (for e.g., WF_6) to concentrate in cold regions whereas small, light molecules (such as H_2) to concentrate in hot regions. Hence, non-isothermal systems could require new closure relationships which, of course, relax to the isothermal one when the temperature is uniform in time and constant in space.

The closure relation that we suggest is the following: sum of the molar fluxes J_i is locally proportional to the gradient of the total molar concentration, i.e.,

$$\sum_{i=1}^{n} J_i = -\alpha \nabla c_{\text{tot}}.$$

With respect to the above mentioned closure relation, we characterize the total molar concentration c_{tot} and the temperature field $T(t,x)$ as solutions to a coupled system of evolution equations. Furthermore, the temperature-dependent flux-gradient relations derived in this paper – see second line of (24) – implies that the product $c_{\text{tot}}T$ is space-independent. Hence the above mentioned closure relation postulated in this paper recovers the standard closure relation – sum of the molar fluxes J_i being locally identically zero – in the isothermal case.

The outline of the paper is as follows: In Section 2.1, we introduce the kinetic model – system of Boltzmann equations for gas mixtures – and present the assumptions made on the Boltzmann collision kernels (Maxwellian molecules). Section 2.2 deals with the scaling considered in this work and the main assumption made on the solutions to the scaled mesoscopic kinetic model. In Section 2.3 we derive the balance laws (mass, momentum and energy) — see Proposition 1. Emphasis is given on computing the coefficients in the balance laws — given in terms of the velocity averages of certain statistical quantities. A formal asymptotic analysis (in the mean free path going to zero limit) is performed in Section 2.4 which culminates in Theorem 2. Section 2.5 deals with the closure relation. Finally, in Section 2.6, we derive some qualitative properties on the total concentration $c_{\text{tot}}(t,x)$ and the temperature field $T(t,x)$.

Please cite this article in press as: H. Hutridurga, F. Salvarani, Maxwell–Stefan diffusion asymptotics for gas mixtures in non-isothermal setting, Nonlinear Analysis (2017), http://dx.doi.org/10.1016/j.na.2017.03.019