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**Mathematical modelling of granular gases
in the context of Grad's Theory and
Rational Extended Thermodynamics**

Author:
Annamaria Pollino

Supervisor:
Prof. Elvira Barbera

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Declaration of Authorship

I, Annamaria Pollino, declare that this thesis titled, "Mathematical modelling of granular gases in the context of Grad's Theory and Rational Extended Thermodynamics" and the work presented in it are my own. I confirm that:

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- Where I have consulted the published work of others, this is always clearly attributed.
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- I have acknowledged all main sources of help.
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*“Non domandarci la formula che mondi possa aprirti
sì qualche storta sillaba e secca come un ramo.
Codesto solo oggi possiamo dirti,
ciò che non siamo, ciò che non vogliamo.”*

Eugenio Montale

UNIVERSITY OF PALERMO

Abstract

Department of Mathematics and Computer Sciences

Doctor of Philosophy

Mathematical modelling of granular gases in the context of Grad's Theory and Rational Extended Thermodynamics

by Annamaria Pollino

Kinetic theory is a discipline introduced by Boltzmann in the late 19th century to study monatomic gas at the microscopic level, introducing a distribution function, which depends on macroscopic variables, such as time and position of particles in space and microscopic variables such as particle velocity. The evolution of the distribution function is defined by the Boltzmann equation from which the macroscopic equations of Euler and Navier-Stokes can be derived.

The theory of Rational Extended Thermodynamics, formulated by Ingo Müller and Tommaso Ruggeri in the last century, deals with the study of non equilibrium phenomena at a macroscopic level, such as shock waves, micro- and nano-flows, second sounds, light scattering, rarefied gases and so on. It consists of a hierarchy of balance laws, where dissipative fluxes are assumed as field variables. The same hierarchy of equations is found in the moment systems of kinetic theory by truncating at an arbitrary order of moments.

There are various points of contact between the two theories. Extended thermodynamics postulates the existence of a law of entropy that imposes conditions of non-negativity for the production of entropy, and kinetic theory also places conditions on the sign of entropic dissipation through the H theorem. Grad's 13-moment theory provides the same phenomenological equations as extended thermodynamics and represents a theoretical validation. It is therefore interesting to study a phenomenon of unbalance for gases from the perspective of kinetic theory and from the point of view of extended thermodynamics, then making comparisons between the results provided by the two theories.

In this thesis, a study is conducted on monatomic granular gases, particles that are subject to inelastic collisions, in which there is no energy conservation. The first case study concerns dilute granular gases, characterized by very spaced particles, where the centers of two colliding particles coincide and in the collision of two particles the effect of nearby particles is neglected. The study is done first by considering a model of differential equations for 13 moments, of which the terms of production are calculated with the method of Grad moments, typical of kinetic theory. Then the same model is derived using the theory of extended thermodynamics and some investigations are conducted on the hyperbolicity region of the system and the convexity of entropy. In addition, spatially homogeneous solutions are studied in the one-dimensional case, comparing in particular the decay of the temperature of the gas to the Haff law. Stationary solutions are also determined in the one-dimensional case.

A more complex case to be considered from the point of view of kinetic theory and extended thermodynamics concerns dense granular gases: particles interact in such a way that in binary collision the effect of other nearby particles cannot be neglected, and the centers of two colliding particles are distinct. A nearly linear model of differential equations for 14 moments is presented and flows and production terms are determined through kinetic theory. The model is then derived in the context of extended thermodynamics for moderately dense gases. This thesis also deepens some biological applications through Extended Thermodynamics. A model of 14 moments is proposed for the study of blood, thought as a mixture, formed by plasma, red blood cells and white blood cells, of which solutions are determined in the linear case, in plane symmetry and cylindrical symmetry. Another biological application regards the evolution of a chronic wasting disease through the definition of a hyperbolic system that predicts finite wave speeds. The linear stability of solutions and the behavior of acceleration waves are investigated.

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Introduction

The aim of the doctoral thesis is the study of some non equilibrium phenomena based on two theories of mathematical physics: Kinetic theory and Rational Extended Thermodynamics.

Kinetic theory is a discipline introduced by Boltzmann in the late 19th century. It deals with the study of gas particle systems at the microscopic level, introducing a non-negative function, $f(x, t, v)$ called distribution function, which depends on macroscopic variables, such as time t and position of particles in space x and microscopic variables such as particle velocity v . The quantity $f(x, t, v)dx dv$ expresses the concentration of gas molecules in the volume element $dx dv$ in the vicinity of the point (x, v) at time t . The evolution of the distribution function is defined by the Boltzmann equation from which the macroscopic equations of Euler and Navier-Stokes can be derived.

The theory of Rational Extended Thermodynamics, formulated by Ingo Müller and Tommaso Ruggeri [Müller and Ruggeri, 2013] in the last century, deals with the study of non equilibrium phenomena at a macroscopic level, such as shock waves [Weiss, 1995], micro- and nano-flows, second sounds, light scattering [Weiss and Müller, 1995] and so on. It consists of a hierarchy of balance laws, where dissipative flows are assumed as field variables. The same hierarchy of equations is found in the moment systems of kinetic theory by truncating at an arbitrary order of moments.

Research in recent decades has been dedicated to the study of granular materials, that is, agglomerates of particles that perform inelastic collisions. Under the hypothesis of driving forces acting on them, these materials exhibit a behavior similar to granular gases, which has led many researchers to study them with the techniques of kinetic theory. A significant contribution to the study of granular materials and to the analogies with granular gases was provided by Campbell [Campbell, 1990] and Goldhirsch [Goldhirsch, 2003]. The study of granular materials allowed to investigate interesting phenomena, such as the formation of hexagonal patterns and kinks in oscillated granular layers [Melo, Umbanhowar, and Swinney, 1995]. Essentially, two lines of research concerning the kinetic theory of granular materials have developed: on the one hand the theory of Chapman Enskog expansion and on the other the method of Grad moments. Both theories aim at solving the nonlinear Boltzmann equation and obtaining the Euler equations, the Navier-Stokes equations and at higher order the Burnett equations. In 1982 Bobylev [Bobylev, 1982] proved that while higher-order approximations of Chapman Enskog theory lead to unstable equations, Grad's method provides stable equations for monatomic gases. Despite this, research has been very prolific in the first field for monatomic gases. The fact that Grad's theory has been less used in monatomic gases may lie within the following limits: it is very difficult to find the terms of production of the balance laws and it is not well known how many nor what moments to choose for the model. Surely both theories have the disadvantage of not having clear boundary conditions. So we can say that initially the research focused on the study of gases based on CE methods. In fact, in [Goldshtein and Shapiro, 1995] Goldshtein and Shapiro determined through CE expansions the Euler equations for granular flows. Brey [Brey et

al., 1998] applied CE theory to derive the Navier Stokes and Fourier equations for dilute granular gases, instead Garzò [Garzó and Dufty, 1999] extended the same study to dense granular gases. Sela et al [Sela, Goldhirsch, and Noskowitz, 1996] defined the distribution function in terms of the number of Knudsen and the coefficient of restitution e , which varies between 0 and 1 and expresses the degree of inelasticity of collisions (for $e=1$ the collision is elastic). Practically limiting themselves to the case of e close to 1, they determined with the CE theory the Burnett relations for a two-dimensional granular gas. Lutsko [Lutsko, 2005] studied the dense granular gases and through the CE expansion obtained to the order zero the homogeneous cooling state while to the first order the relations of Navier Stokes and Fourier. Garzò et al [Kremer, Santos, and Garzó, 2014] determined the Burnett relations for a smooth granular gas for different values of the restitution coefficient. However, it must be said that the research then used the techniques of Grad's theory for the study of granular gases. The first to apply it to dense and granular gases were Jenkins and Richman who in [Jenkins and Richman, 1985a] provided a model of 13 moments, while in [Jenkins and Richman, 1985b] a model of 16 moments, in which they also described the rotation of two-dimensional particles during the collision. Bisi et al [Bisi, Spiga, and Toscani, 2004] investigated the behavior of weakly inelastic gas in 1 dimension. Kremer et al [Kremer and Marques Jr, 2011] derived a 14 moments model, based on Grad theory, for a dilute granular gas, they analyzed the homogeneous cooling state related to the Haff law and studied the stability of a linearized model with 13 moments. Gupta and Torrilhon [Gupta and Torrilhon, 2012] idealized a computational method to determine the production terms of Grad models for monatomic gas, mixtures of monatomic gases and granular gas. In [Gupta, Shukla, and Torrilhon, 2018a] Gupta et al derived a 26 moments theory for dilute granular gas through Grad method and found constitutive relations for stress tensor and heat flux. They also studied the stability analysis of the model with eigenmodes.

Although kinetic theory deals with physical phenomena from a microscopic point of view and thermodynamics from a macroscopic point of view, there are many points of contact between the two theories. Thermodynamics, particularly the second law, predicts the arrow of time, according to which thermodynamic processes in nature occur irreversibly and this has been proven by Boltzmann through the H theorem on entropic dissipation. Parallel to kinetic theory, in the last seventy years, starting from the works of Onsager, Eckart, Meixner, Prigogine and others, Extended Thermodynamics has developed as a systematic thermodynamic theory of unbalance. The thermodynamics of irreversible processes have been used in the study of various phenomena of the non equilibrium such as mass diffusion and viscous fluids [Müller and Ruggeri, 2013], heat conduction [Donato and Ruggeri, 2000], chemical reactions [Kremer and Müller, 1998], electrical conduction etc.

One limitation that raises classic thermodynamic theory is that it is based on models of parabolic differential equations that admit wave solutions at infinite velocities. The rational extended thermodynamics was conceived to overcome this limit. In fact, it allows to define for the study of rarefied gases or gases far from equilibrium models of quasi-linear hyperbolic differential equations, which guarantee the finite velocity of waves. The state of the gas under consideration is defined not only by density, velocity and temperature, but is extended to stress tensor and heat flux which are no longer constitutive variables as in classical thermodynamics, but they become fields, for which it is necessary to assign balance laws. A further advantage of extended thermodynamics models is that they guarantee the existence, uniqueness of the solutions and their continuous dependence on the initial data.

However, the models in question are not closed. To determine the constituent variables, universal physical principles are adopted: the principle of Galilean invariance and the principle of entropy. The Galilean invariance allows the decomposition of moments, fluxes and productions in the convective and non convective parts. The principle of entropy postulates the existence of a convex function, the density of entropy that satisfies the law of conservation of entropy. This is an additional law that must be verified by the field variables. To this end, Lagrange multipliers are introduced according to the theory elaborated by Liu [Liu, 1972, Ruggeri and Strumia, 1981] that allow the assumption of the balance laws as constraints for the law of entropy.

Another point of contact between Extended Thermodynamics and Kinetic Theory is that field variables used in Extended Thermodynamics [Müller and Ruggeri, 2013] are the moments of the distribution function and the phenomenological equations of Extended Thermodynamics coincide with those obtained with the Grad's method for 13 moments. Extended Thermodynamics has also been applied to the study of polyatomic gases by defining a structure model [Ruggeri and Sugiyama, 2015, Ruggeri and Sugiyama, 2021] with two hierarchies of moments: one for mass and the other for energy. It has been shown that Rational Extended Thermodynamics (RET) can describe processes where rapid time changes or when a strong deviation from equilibrium occur. On the other hand models with more than two hierarchies of moments are newly emerged [Arima et al., 2021b]. In fact, it has been shown that the field equations of RET can describe a range various non-equilibrium phenomena such as light shattering, sound waves, heat waves, structure of shock waves [Müller and Ruggeri, 2013, Ruggeri and Sugiyama, 2015, Ruggeri and Sugiyama, 2021]. RET has been applied to monatomic gases [Müller and Ruggeri, 2013] and mixtures [Müller and Ruggeri, 2013, Ruggeri and Sugiyama, 2015, Barbera and Brini, 2011b, Barbera and Brini, 2011a, Barbera and Brini, 2014] with many interesting results. Recently, RET has been generalized to dense and rarefied polyatomic gases both in the classical [Ruggeri and Sugiyama, 2015; Ruggeri and Sugiyama, 2015; Carrisi, Montisci, and Pennisi, 2013; Arima et al., 2012; Arima et al., 2021b] and in the relativistic framework [Ruggeri and Sugiyama, 2021; Pennisi and Ruggeri, 2017; Arima et al., 2022; Arima and Carrisi, 2023], for metal electrons [Barbera and Brini, 2019; Barbera and Brini, 2021], to quantum systems [Trovato, 2014, Brini and Seccia, 2022; Brini and Seccia, 2023], and also for biological systems [Barbera, Curro, and Valenti, 2015; Consolo et al., 2022; Consolo, Currò, and Valenti, 2020; Consolo and Grifó, 2022], providing relevant results and good agreement with experimental data.

As has been deduced in the work [Müller and Ruggeri, 2004], even when studying a rather simple physical phenomenon, such as the stationary heat conduction in a monatomic gas, the differences between classical thermodynamics and extended thermodynamics are evident. These differences become more marked in the case of curved domains [Müller and Ruggeri, 2004] where the authors studied a rarefied gas at rest between two circular coaxial cylinders. Precisely they noted that the normal components of stress tensor vanish as in classical thermodynamics and this implies that Fourier's law is not valid. Barbera et al. [Barbera and Müller, 2006] also studied the gas behavior between two rotating coaxial cylinders, showing that no rigid rotation is compatible with Grad's theory unlike Navier Stokes and Fourier theory. The differences between extended and classical thermodynamics in the study of a rarefied gas at rest between two confocal elliptical cylinders were also shown in [Barbera and Müller, 2008]. Then, the analysis of stationary heat transfer problems was extended to general 3D symmetric domains [Barbera and Brini, 2010; Barbera, Brini,

and Valenti, 2012]. All these studies lead to the general idea that, the differences between the stationary solutions of classical and extended thermodynamics increase when the geometry of the problem becomes more complex and further from the planar one. Meanwhile, other authors studied the solution of 13-moment extended thermodynamics when a flow is introduced. In particular, Marques Jr. and Kremer [Marques Jr and Kremer, 2001] investigated the planar Couette flow, whereas Gramani Cumin et al. [Cumin, Kremer, and Sharipov, 2002] (see also the references therein) investigated the non-isothermal cylindrical Couette flow with a tangential velocity. It was shown that the nonlinear equations of 13-moment extended thermodynamics are already able to predict some differences from the classical thermodynamics which are in agreement with the expectation of the kinetic theory. More recently 3D flows are also investigated [Barbera and Brini, 2017; Barbera and Brini, 2018] and for different gases where the dynamic pressure becomes more evident [Arima et al., 2014; Barbera, Brini, and Sugiyama, 2014].

The main topic of the PhD thesis is the investigation of rarefied granular gases and dense granular gases on the basis of Kinetic Theory and Extended Thermodynamics. Quasilinear models, comprised of 13 or 14 partial differential equations for 13 or 14 moments respectively, are presented and with the techniques of kinetic theory the fluxes and source terms expressing the dense character of the gas are determined. These models are then defined in the context of Extended thermodynamics and the values of bulk viscosity and thermal conductivity of Navier Stokes and Fourier laws respectively are recovered. In addition, models are integrated and various numerical applications on spatially homogeneous solutions are conducted. One of the advantages of these models is that they can be used in many fields of research. For example, granular gases have a similar behavior to granular materials. This has meant that the research of granular gases has extended to the study of many physical applications that concern granular materials, such as the industrial transport of cereals, ores, pharmaceuticals, granular snow avalanches, rock debris slides and underwater sediment slumps. In this thesis we also carried out two biological applications, through models of quasilinear and hyperbolic systems of partial differential equations, defined in the context of Extended Thermodynamics. The first is inspired by a classic model elaborated by Dimitri Gidaspow [Gidaspow and Huang, 2009] in which he studies the behavior of red blood cells in narrow vessels. We define a new model adding moments and balance laws and evaluate the concentrations and velocity of red blood cells, finding accordance with the paper [Gidaspow and Huang, 2009] and some new results about the stress tensor and heat flux, thanks to the more precision of Extended Thermodynamics.

The second biological application is about a reaction-diffusion model [Sharp and Pastor, 2011] in order to investigate the evolution of mad cow disease that affects various animal species by ingestion of foods, containing misfolded proteins called prions. Reaction-diffusion models, that involve the Fick law for the diffusion aspect, are parabolic and so they predict the diffusion of the biological population at a infinity speed. Here we substitute the Fick law with the balance laws of Extended Thermodynamics in order to recover coherent finite speed of diffusion.

The thesis is divided as follows. The main objective of Chapter 1 is to lay the foundations of two kinetic models for granular dense gas, i.e. high dense gas molecules, that are subject to inelastic collisions. The first was developed by Jenkins and Savage [Jenkins and Savage, 1983] and the second by Jenkins and Richman [Jenkins and Richman, 1985a]. These models of kinetic theory provide the balance laws for density, velocity and energy and allow to compute the specific forms for the mean fluxes of momentum and energy and the mean rate at which energy is lost in collisions.

In Chapter 2 we investigate the behavior of rarefied granular gas in the context of Extended Thermodynamics and derive a quasi linear system of differential equations for 13 moments [Barbera E, 2023, Barbera and Pollino, 2023c]. The model has to be closed by constitutive relations that are determined by invoking universal physical principles, such as the entropy law and the principle of Galilean invariance. We determine linear solutions in two cases: spatially homogeneous solutions and stationary solutions in one dimensional space. We also show that these solutions are found in the acceptable regions of the model, that is, in the region where the model is hyperbolic, which guarantees the existence and uniqueness of the solutions, continuous dependence on initial data and the propagation of waves at finite speed and also in the region where entropy production is non-negative.

In Chapter 3 [Barbera and Pollino, 2023d] we focus on dense granular gases: the particles have positions and velocities that depend on each other and the collisions are inelastic. The positions of the centers of two colliding particles are distinguished, and in collision, the position of the two particles is affected by the presence of neighboring particles. The phenomenon of transfer of particle properties and transport have to be considered. Using the techniques of kinetic theory we define a fourteen moments model for dense granular gas and we determine fluxes associated with transport and fluxes associated with transfer. Precisely adopting approximate linear formulas [Jenkins and Richman, 1985a], we compute all the fluxes and source for each balance equation. Chapter 4 is devoted to the determination of a 14 moments model for moderately dense granular gas in the context of Extended Thermodynamics [Barbera and Pollino, 2023e]. Physical universal principles are invoked to close the system and production terms are recovered by comparison with those obtained in the previous chapter. Chapter 5 and Chapter 6 are dedicated to biological applications of Extended Thermodynamics. In Chapter 5 we define a 14 moments model for blood flow, regarded as a mixture comprised of plasma, red blood cells and white blood cells. We base on the paper [Barbera and Pollino, 2022, Barbera and Pollino, 2023b] and we define a quasi linear differential model following the structure of the two hierarchies of moments, elaborated in [Ruggeri and Sugiyama, 2015]. Aim of this chapter is the investigation of the Fåhræus-Linqvist effect, that is the migration of red blood cells from the wall to the center of narrow vessels. Chapter 6 is devoted to the investigation of a chronic wasting disease through a reaction-diffusion model [Barbera and Pollino, 2023a, Sharp and Pastor, 2011]. We study the linear stability of the equilibrium solutions and analyze the propagation of acceleration waves, that are expected to occur at finite velocity.

Chapter 1

A Kinetic Model of 13 moments for granular gas

1.1 Introduction

Based on experiments conducted by Savage and others, [Savage and Mckeown, 1983; Savage and Sayed, 1984], it was noticed that granular materials, composed of spherical, identical, dense and nearly elastic particles have a behavior similar to that of dense gases. In fact it has been observed that in the granular flows collisions occur instantaneously between pairs of spheres.

This has led many researchers to study granular materials by applying the theory of non-ordinary kinetic equilibrium theory, developed by Chapman and Cowling for dense gas [Chapman and Cowling, 1990]. The drawback of this approach lies in the fact that in collisions between granular particles the kinetic energy is not conserved but this limit has been overcome by adapting the kinetic theory ad hoc to the class of granular materials.

Research was carried out in order to investigate the evolution of planetary rings, the industrial transport of cereals, ores and pharmaceuticals and also geophysical phenomena such as, granular snow avalanches, rock debris slides and underwater sediment slumps.

Models of kinetic theory allow to determine the balance laws for density, velocity and energy and to compute the specific forms for the mean fluxes of momentum and energy and the mean rate at which energy is lost in collisions.

The main objective of this introductory chapter is to lay the foundations of two kinetic models for granular dense gas, i.e. high dense gas molecules, that are subject to inelastic collisions. The first was developed by Jenkins and Savage [Jenkins and Savage, 1983] and the second by Jenkins and Richman [Jenkins and Richman, 1985a]. Going into detail, in 1983 Jenkins and Savage [Jenkins and Savage, 1983] studied an idealized material comprised of identical, smooth, nearly elastic, spherical particles, in which the particles interact only through binary collisions with their neighbors. They formulated the probability of binary collisions in the following form

$$f^{(2)}(c_1, r_1, c_2, r_2) = g(r_1, r_2) f^{(1)}(c_1, r_1) f^{(1)}(c_2, r_2),$$

where c_i and r_i are the velocity and the position respectively of the i particle, $f^{(2)}(c_1, r_1, c_2, r_2)$ is the pair distribution function, $f^{(i)}(c_i, r_i)$ the single particle velocity distribution function and $g(r_1, r_2)$ a radial distribution function for dense gases. This allowed them to derive local expressions for the balance laws and integral expressions for the stress, energy flux and energy dissipation.

In 1984 Jenkins and Richman [Jenkins and Richman, 1985a] extended the Grad's method of moments [Grad, 1958] from the dilute system of elastic particles to dense

system of inelastic particles. They determined analytical expressions for the collisional fluxes and the collisional productions of the velocity moments, keeping of the fact that in dense gases colliding particles have different positions in space and are affected by the presence of other nearby particles. Finally they provided the balance laws of the Grad's 13 moment system.

1.2 Kinetic theory for a dense system of nearly elastic spheres

1.2.1 Setting

Following Jenkins and Savage [Jenkins and Savage, 1983], we consider a dense system of macroscopic particles that are identical spheres of diameter σ and mass m . We suppose that the collisions between them are binary but nearly elastic. Indicating with c_1 and c'_1 the velocities of the particle "1" before and after the collisions and with c_2 and c'_2 those of the particle "2", one has, for the balance of linear momentum,

$$\begin{aligned} mc'_{1i} &= mc_{1i} - J_i, \\ mc'_{2i} &= mc_{2i} + J_i, \end{aligned} \quad (1.1)$$

where J_i is the impulse of the force exerted by particle "1" upon particle "2" during collision. If $\mathbf{g} = \mathbf{c}_1 - \mathbf{c}_2$ and $\mathbf{g}' = \mathbf{c}'_1 - \mathbf{c}'_2$ are the relative velocities of the centers of the spheres immediately before and after the collisions and \mathbf{k} is the unit vector directed from the center of particle "1" to the center of "2" at contact, we suppose that the component normal to the plane of contact of the particles is related to the component normal prior to collision by

$$(\mathbf{g}' \cdot \mathbf{k}) = -e (\mathbf{g} \cdot \mathbf{k}) \quad (1.2)$$

where e is the so-called restitution coefficient, with $0 \leq e \leq 1$. When $e = 1$, the relative velocities are reversed upon collision and energy is conserved. Values of e less than 1 indicate dissipation of energy.

By combination of (1.1) and (1.2) one gets

$$\begin{aligned} c'_{1i} &= c_{1i} - \frac{1}{2} (1 + e) (\mathbf{g} \cdot \mathbf{k}) k_i, \\ c'_{2i} &= c_{2i} + \frac{1}{2} (1 + e) (\mathbf{g} \cdot \mathbf{k}) k_i, \end{aligned} \quad (1.3)$$

which describe the relations of the velocities of the particles "1" and "2" before and after the collision.

By combinations of (1.3), it is easy to obtain some relations that will be useful later in the determination of fluxes and productions, that are

$$\begin{aligned} c'_{1i} c'_{1j} - c_{1i} c_{1j} &= \frac{1}{2} (1 + e) (\mathbf{g} \cdot \mathbf{k}) \left[\frac{1}{2} (1 + e) (\mathbf{g} \cdot \mathbf{k}) k_i k_j - (k_i c_{1j} + k_j c_{1i}) \right], \\ c'_{1i} c'_{1j} c'_{1p} - c_{1i} c_{1j} c_{1p} &= -\frac{1}{2} (1 + e) (\mathbf{g} \cdot \mathbf{k}) \left[3k_i c_{1j} c_{1p} - \frac{3}{2} (1 + e) (\mathbf{g} \cdot \mathbf{k}) k_i k_j c_{1p}^1 + \right. \\ &\quad \left. + \frac{1}{4} (1 + e)^2 (\mathbf{g} \cdot \mathbf{k})^2 k_i k_j k_p \right], \\ c'_{1l} c'_{1l} c'_{1s} c'_{1s} - c_{1l} c_{1l} c_{1s} c_{1s} &= -2 (1 + e) (\mathbf{g} \cdot \mathbf{k}) \left[k_l c_{1l} c_{1s} c_{1s} - \frac{1}{2} (1 + e) (\mathbf{g} \cdot \mathbf{k}) (k_l c_{1l})^2 + \right. \\ &\quad \left. - \frac{1}{4} (1 + e) (\mathbf{g} \cdot \mathbf{k}) c_{1s} c_{1s} + \frac{1}{4} (1 + e)^2 (\mathbf{g} \cdot \mathbf{k})^2 k_l c_{1l} - \frac{1}{32} (1 + e)^3 (\mathbf{g} \cdot \mathbf{k})^3 \right]. \end{aligned} \quad (1.4)$$

Similarly it is possible to obtain other relations, setting $\Delta\psi = \psi'_1 + \psi'_2 - \psi_1 - \psi_2$:

$$\begin{aligned}\Delta(c_i c_j) &= \frac{1}{2} (1 + e) (\mathbf{g} \cdot \mathbf{k}) [(1 + e) (\mathbf{g} \cdot \mathbf{k}) k_i k_j - (k_i g_j + k_j g_i)], \\ \Delta(c_i c_j c_k) &= 3Q_i \Delta(c_j c_k), \\ \Delta(c^4) &= \frac{1}{8} (1 + e)^4 (\mathbf{g} \cdot \mathbf{k})^4 - \frac{1}{2} (1 + e)^3 (\mathbf{g} \cdot \mathbf{k})^4 + \\ &+ (1 + e)^2 (\mathbf{g} \cdot \mathbf{k})^2 \left[Q^2 + \frac{1}{4} g^2 + 2 (\mathbf{Q} \cdot \mathbf{k})^2 + \frac{1}{2} (\mathbf{g} \cdot \mathbf{k})^2 \right] + \\ &- (1 + e) (\mathbf{g} \cdot \mathbf{k}) \left[\frac{1}{2} (\mathbf{g} \cdot \mathbf{k}) g^2 + 2 (\mathbf{g} \cdot \mathbf{k}) Q^2 + 4 (\mathbf{g} \cdot \mathbf{Q}) (\mathbf{Q} \cdot \mathbf{k}) \right]\end{aligned}\quad (1.5)$$

with $Q_i = \frac{1}{2} (c_{1i} + c_{2i})$, that is the velocity of the center of mass of the two particles. If we consider the kinetic energy $E = \frac{1}{2} m c^2$ and apply (1.5), we obtain:

$$\Delta E = -\frac{1}{4} m (1 - e^2) (\mathbf{g} \cdot \mathbf{k})^2, \quad (1.6)$$

that confirms the conservation of kinetic energy when $e = 1$.

1.2.2 Distribution function

We define the two particle configurational distribution function, $n^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$, such that $n^{(2)}(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2$ is the probable number of pairs of particles, each in the volume $d\mathbf{r}_1$ and $d\mathbf{r}_2$, centered at \mathbf{r}_1 and \mathbf{r}_2 respectively. Its analytical formulation, when the particle flow is homogeneous, is given by

$$n^{(2)}(\mathbf{r}_1, \mathbf{r}_2) := g_0(d) n^2, \quad (1.7)$$

where n is the uniform number density of particles, $d = |\mathbf{r}_1 - \mathbf{r}_2|$ and $g_0(d)$ a radial distribution function. An expression of g_0 for a fluid of identical hard spheres, whose solid volume fraction $\nu = \frac{1}{6} \pi n \sigma^3$, is numerically determined by Carnahan and Starling:

$$g_0(\nu) = \frac{1}{1 - \nu} + \frac{3\nu}{2(1 - \nu)^2} + \frac{\nu^2}{2(1 - \nu)^3}. \quad (1.8)$$

If $f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2, t)$ is the pair distribution function, with $f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2, t) d\mathbf{c}_1 d\mathbf{r}_1 d\mathbf{c}_2 d\mathbf{r}_2$ the probable number of pairs of particles located in the volumes $d\mathbf{r}_1, d\mathbf{r}_2$, centred at \mathbf{r}_1 and \mathbf{r}_2 , and having velocities $\mathbf{c}_1, \mathbf{c}_2$, centred in the ranges $d\mathbf{c}_1, d\mathbf{c}_2$, at time t , then the probable number of binary particle collisions, $n^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$ is obtained by integrating $f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2, t)$ on all velocities:

$$\int \int f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2, t) d\mathbf{c}_1 d\mathbf{c}_2 = n^{(2)}(\mathbf{r}_1, \mathbf{r}_2, t). \quad (1.9)$$

Given any property $\psi(\mathbf{c}_1, \mathbf{c}_2)$, its mean $\langle \psi \rangle$ is determined by

$$\langle \psi \rangle = \frac{1}{n} \int \int \psi(\mathbf{c}_1, \mathbf{c}_2) f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2, t) d\mathbf{c}_1 d\mathbf{c}_2. \quad (1.10)$$

Maxwellian transport equation for any property of a particle $\psi(\mathbf{c})$ is given by

$$\frac{\partial}{\partial t} \langle n\psi \rangle = n \langle D\psi \rangle - \nabla \cdot \langle n\mathbf{c}\psi \rangle + C(\psi) \quad (1.11)$$

where $D\psi = \frac{dc}{dt} \cdot \frac{\partial\psi}{\partial c} = \frac{1}{m} \mathbf{F} \cdot \frac{\partial\psi}{\partial c}$ and \mathbf{F} is the external force acting on a particle. The change of ψ at an instant dt and in a fraction of volume dr , is caused by three factors: the change in velocity represented by $D\psi$, the passage of the particles entering and leaving dr , indicated by the divergence $\nabla \cdot \langle n\mathbf{c}\psi \rangle$ and the collisions $C(\psi)$ that take place between particles. Now, we develop some expressions for the collision term $C(\psi)$. If we consider two particles colliding with velocities \mathbf{c}_1 and \mathbf{c}_2 and causing the property ψ to vary from value ψ_2 to value ψ'_2 , the expression of the change of ψ is determined by [Jenkins and Savage, 1983] in the following way:

$$C(\psi) = \int \int \int (\psi'_2 - \psi_2) f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2. \quad (1.12)$$

We specify that the triple integrals from here on are calculated on the domain $\mathbf{g} \cdot \mathbf{k} > 0$, which is the one in which it is considered admissible collision. It is possible to get a similar formula when ψ property varies from ψ_1 to ψ'_1 and to recover the total variation of ψ as follows:

$$C(\psi) = -\nabla \cdot \theta(\psi) + \chi(\psi), \quad (1.13)$$

where

$$\theta(\psi) = -\frac{1}{2} \sigma \int \int \int \mathbf{k} (\psi'_1 - \psi_1) f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2, \quad (1.14)$$

$$\chi(\psi) = \frac{1}{2} \int \int \int \mathbf{k} (\psi'_1 + \psi'_2 - \psi_1 - \psi_2) f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2. \quad (1.15)$$

So, the Maxwellian equation can be reviewed as

$$\frac{\partial}{\partial t} \langle n\psi \rangle = n \langle D\psi \rangle - \nabla \cdot \langle n\mathbf{c}\psi \rangle - \nabla \cdot \theta(\psi) + \chi(\psi). \quad (1.16)$$

Now, we show how we derive from this equation balance laws of mass, momentum and energy. If we set $\psi = mn = \rho$, we obtain the conservation law of mass:

$$\dot{\rho} = \rho \nabla \cdot \mathbf{u}, \quad (1.17)$$

where \mathbf{u} is the mean velocity and the dot stands for the time derivative with respect to the mean motion, $\frac{\partial}{\partial t} + u_i \frac{\partial}{\partial r_i}$ and \mathbf{u} . If $\psi = mc$, we recover the local form of the balance of linear momentum:

$$\rho \dot{\mathbf{u}} = -\nabla \cdot \langle \rho \mathbf{C} \otimes \mathbf{C} \rangle - \nabla \cdot \mathbf{P} + n\mathbf{F}, \quad (1.18)$$

where \otimes is the tensor product, $\mathbf{C} = \mathbf{c} - \mathbf{u}$ and \mathbf{P} is the pressure tensor, given by

$$\mathbf{P} = -\frac{1}{2} m \sigma \int \int \int (\mathbf{c}'_1 - \mathbf{c}_1) \otimes \mathbf{k} f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2. \quad (1.19)$$

Finally, taking $\psi = \frac{1}{2} mc^2$ gives the local form of the balance of energy:

$$\frac{3}{2} \rho \dot{T} = -\nabla \cdot \langle \frac{1}{2} \rho \mathbf{C}^2 \mathbf{C} \rangle - \text{tr}(\nabla \mathbf{u} \langle \rho \mathbf{C} \otimes \mathbf{C} \rangle) - \nabla \cdot \mathbf{q} - \text{tr}(\mathbf{P} \nabla \mathbf{u}) - \gamma, \quad (1.20)$$

where $T = \frac{1}{3} \langle \mathbf{C}^2 \rangle$,

$$\mathbf{q} = -\frac{1}{4} m \sigma \int \int \int \mathbf{k} (\mathbf{C}'_1{}^2 - \mathbf{C}_1^2) f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2 \quad (1.21)$$

and the collisional rate of dissipation per unit volume γ is given by

$$\gamma = -\frac{1}{4}m\sigma \int \int \int (\dot{c}_1'^2 + \dot{c}_2'^2 - c_1^2 - c_2^2) f^{(2)}(c_1, r_1, c_2, r_2) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} dc_1 dc_2. \quad (1.22)$$

In collisions between dense gases it is possible to neglect the transport phenomenon of the property ψ , while the transfer of the property ψ due to the collision must be considered. So we can overlook the terms $\nabla \cdot \langle \rho \mathbf{C} \otimes \mathbf{C} \rangle$ related to (1.18) and terms $-\nabla \cdot \langle \frac{1}{2} \rho \mathbf{C}^2 \mathbf{C} \rangle - \text{tr}(\nabla \mathbf{u} \langle \rho \mathbf{C} \otimes \mathbf{C} \rangle)$ related to (1.20).

In the case of non homogeneous flow, collisions between approaching particles are more likely than those between moving away particles. This means that the pair distribution function manifests a collisional anisotropy. So the best way to represent it would be to determine it as the solution of the Boltzmann evolution equation. But given the difficulty of calculation, Jenkins and Savage [Jenkins and Savage, 1983] prefer to define a form of the pair distribution function, similar to that derived from Chapman and Cowling as an approximate solution of the Boltzmann equation. They represent the distribution function in the following way:

$$f^{(2)}(c_1, r_1, c_2, r_2) = g(r_1, r_2) f^{(1)}(c_1, r_1) f^{(1)}(c_2, r_2) \quad (1.23)$$

where

$$f^{(1)}(c_i, r_i) = n_i \left(\frac{1}{2\pi T_i} \right)^{\frac{3}{2}} \exp \left[-\frac{(c_i - u_i)^2}{2T_i} \right] \quad (1.24)$$

is the single particle velocity distribution function for each particle i , expressed as Maxwellian about the mean velocity and

$$g(r_1, r_2) = g_0 \left[1 - \frac{\alpha \mathbf{k} \cdot (\mathbf{u}_2 - \mathbf{u}_1)}{(\pi T)^{\frac{1}{2}}} \right] \quad (1.25)$$

is a normalized pair distribution function for the anisotropy case, with α a generic function of v . So we get the pair distribution function at collision, that contains the mean fields n, \mathbf{u} and T :

$$f^{(2)}(c_1, r_1, c_2, r_2) = g_0 \left(\frac{1}{2\pi} \right)^3 \frac{n_1 n_2}{(T_1 T_2)^{\frac{3}{2}}} \left[1 - \frac{\alpha \mathbf{k} \cdot (\mathbf{u}_2 - \mathbf{u}_1)}{(\pi T)^{\frac{1}{2}}} \right] \exp \left[-\left[\frac{(c_1 - u_1)^2}{2T_1} + \frac{(c_2 - u_2)^2}{2T_2} \right] \right]. \quad (1.26)$$

We adopt the expansion of the pair distribution function in terms of a Taylor series about the point \mathbf{r} in the collision integrals (1.19), (1.21) and (1.22), in order to recover the constitutive relations [Jenkins and Savage, 1983]:

$$\gamma = \frac{k(1-e)}{2\sigma^2} \left[12T - (3\pi + 4\alpha)\sigma \left(\frac{T}{\pi} \right)^{\frac{1}{2}} (\text{tr} \mathbf{D}) \right], \quad (1.27)$$

$$\mathbf{q} = -k \nabla T, \quad (1.28)$$

$$\mathbf{P} = \pi^{\frac{1}{2}} k \sigma^{-1} T^{\frac{1}{2}} \mathbf{I} - \frac{1}{5} k (2 + \alpha) [(\text{tr} \mathbf{D}) \mathbf{I} + 2\mathbf{D}] \quad (1.29)$$

where

$$k = 2\rho v g_0 \sigma (1+e) \left(\frac{T}{\pi} \right)^{\frac{1}{2}}, \quad 2\mathbf{D} = \nabla \mathbf{u} + (\nabla \mathbf{u})^T.$$

We observe that the structure of the heat flux and the pressure tensor, here obtained,

are similar to those, computed by Chapman and Cowling in [Chapman and Cowling, 1990].

1.2.3 An explanatory application

We consider two parallel plates at fixed distance L , in relative motion along the horizontal direction. We are interested to investigate the stationary shear flow between the two plates, where the mean velocity is only horizontal. So we define a rectangular Cartesian system, made of x and y axes and we suppose that the density ρ , the non-vanishing x -component u of the mean velocity and the specific energy T depend only on the component y . The conservation of mass (1.17) is identically verified. The balance law for momentum (1.18) provides the following relations:

$$0 = -\frac{\partial P_{xy}}{\partial y}, \quad (1.30)$$

$$0 = -\frac{\partial P_{yy}}{\partial y} - \rho G, \quad (1.31)$$

where G is the gravitational acceleration. The balance law for specific energy (1.20) reduces to

$$0 = -\frac{\partial q_y}{\partial y} - P_{xy} \frac{\partial u}{\partial y} - \gamma. \quad (1.32)$$

Employing the constitutive relations (1.19), (1.21) and (1.22), we obtain: the component of the pressure tensor

$$P_{xy} = -\frac{1}{5}k(2 + \alpha) \frac{\partial u}{\partial y}, \quad (1.33)$$

$$P_{yy} = \pi^{\frac{1}{2}} k \sigma^{-1} T^{\frac{1}{2}}, \quad (1.34)$$

the heat flux

$$q_y = -k \frac{\partial T}{\partial y}, \quad (1.35)$$

and the dissipation

$$\gamma = 6\sigma^{-2}(1 - e)kT. \quad (1.36)$$

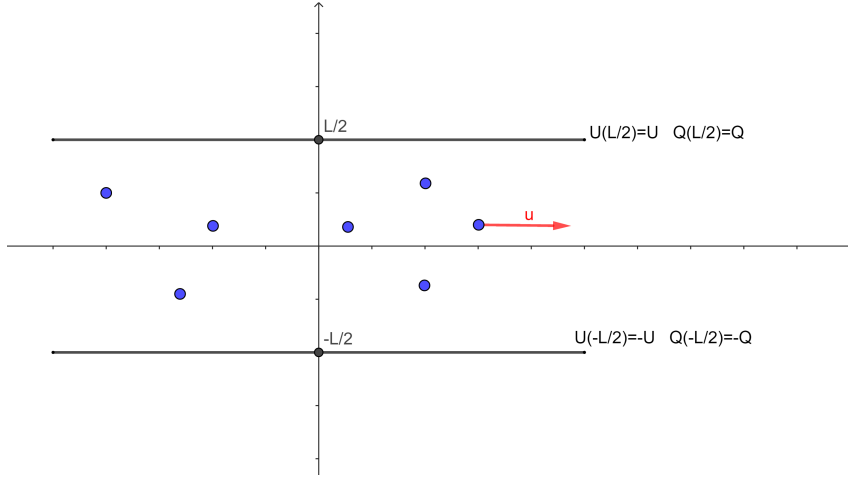
The presence of gravity makes the flow not symmetrical. In addition, when shear rates are very high, vertical forces prevail over weight forces. Therefore it is convenient to study the symmetrical case where gravity is neglected. Let us assume that the Cartesian coordinate system has origin at the center of the flow and adopt as boundary conditions for the mean velocity and the heat flux:

$$u\left(\frac{L}{2}\right) = -u\left(-\frac{L}{2}\right) = U, \quad (1.37)$$

$$q\left(\frac{L}{2}\right) = -q\left(-\frac{L}{2}\right) = Q. \quad (1.38)$$

We integrate the horizontal component of the linear momentum (1.30) and then, using the constitutive relation (1.33), we obtain:

$$\frac{1}{5}k(2 + \alpha) \frac{\partial u}{\partial y} = S, \quad (1.39)$$



where S represents the shear stress applied to the flow at the top plate. Then, if we replace the local value of density ρ by its constant mean value $\bar{\rho}$, we are able to integrate the normal component of linear momentum (1.31), in which gravity is neglected. Finally we obtain, employing the constitutive relation (1.34), the following result:

$$\pi^{\frac{1}{2}} k \sigma^{-1} T^{\frac{1}{2}} = N, \quad (1.40)$$

where N is the normal stress throughout the flow. We determine k from (1.40), $\frac{\partial u}{\partial y}$ from (1.39) and combining the equation (1.32) with the constitutive relations (1.35) and (1.36), we get after some easy computations:

$$\ddot{w} + \lambda w = 0, \quad (1.41)$$

where $w = T^{\frac{1}{2}}$, a dot stands for the derivative with respect to the adimensional vertical coordinate $s = \frac{y}{L}$ and

$$\lambda = \left(\frac{L}{\sigma}\right)^2 \left[\frac{5\pi}{2(2+\alpha)} \left(\frac{S}{N}\right)^2 - 3(1-e) \right]. \quad (1.42)$$

We study the case $\lambda = 0$, in which the specific energy is uniform and there is no heat flux through the boundaries. Using (1.39) and (1.40), together with the boundary condition (1.37) and the equation (1.42), we get the relation between T and the shear rate $2\frac{U}{L}$:

$$T^{\frac{1}{2}} = 2 \left[\frac{2+\alpha}{30(1-e)} \right]^{\frac{1}{2}} \frac{\sigma U}{L}. \quad (1.43)$$

Since k is proportional to $T^{\frac{1}{2}}$, from (1.40) and (1.39) we can conclude that the normal stress N and the shear stress S are proportional to the square of the shear rate $2\frac{U}{L}$. Moreover the term $\frac{\sigma U}{LT^{\frac{1}{2}}}$ depends on the restitution coefficient e and α . We decided to focus on nearly elastic particles because in this case and when e is close to 1, the ratio $\frac{\sigma U}{LT^{\frac{1}{2}}}$ and the anisotropic term $g(\mathbf{r}_1, \mathbf{r}_2)$ of the pair distribution function $f^{(2)}$ in (1.25) are both small.

The study can be further deepened by investigating the case in which λ is not zero and those in which gravity is not neglected. But in the latter case we obtain a linear differential equation that has for solutions Bessel functions of imaginary order and imaginary arguments, difficult to treat. See for more details [Jenkins and Savage,

1983].

1.3 Kinetic theory for a dense system of inelastic particles

We present the main results of the paper [Jenkins and Richman, 1985a], about a dense gas system, composed of inelastic spherical particles. We assume the same setting as in the previous section and suppose that the spatial gradients of the unknown fields, i.e. density, ρ , velocity, u_i , and temperature, T are small so as to neglect the terms of the second order. Let $f^{(1)}(\mathbf{c}, \mathbf{r}, t)$ the single particle distribution function, where \mathbf{c} is the velocity of the particle, \mathbf{r} its position and t time. Let $f^{(2)}(\mathbf{c}_1, \mathbf{r}_1, \mathbf{c}_2, \mathbf{r}_2)$ the pair distribution function that expresses the probability of collisions between two particles, where \mathbf{c}_i and \mathbf{r}_i are respectively the velocity and the position of the generic $i = 1, 2$ particle. Using an approximation of the velocity distribution function for each single particle, $f^{(1)}$, the parts of the pressure tensor, P_{ij} , and heat flux, q_i , due to the transport of momentum and energy between collisions, are determined. Instead, an appropriate approximation of the pair distribution function, $f^{(2)}$, allows to compute the parts of the pressure tensor and heat flux and the energy dissipation, γ , due to the transfer of momentum and energy during collisions. The constitutive relations together with the balance equations are therefore used to determine the unknown fields.

1.3.1 Balance laws

Let $\psi(\mathbf{C})$ the property of a particle, with $\mathbf{C} = \mathbf{c} - \mathbf{u}$ the relative velocity. The collisional rate of change per unit volume, $C(\psi)$ of the property $\psi(\mathbf{C})$, represents the integral over all possible binary collisions of the change of ψ multiplied by the probable frequency of the collision, like the expression (1.12), that we determined in the previous section. Let $f^{(2)}(\mathbf{c}_1, \mathbf{r}, \mathbf{c}_2, \mathbf{r} + \sigma\mathbf{k})$ the pair distribution function regarding two particles such that one is located at the position \mathbf{r} and with velocity \mathbf{c}_1 and the second has the position $\mathbf{r} + \sigma\mathbf{k}$ and velocity \mathbf{c}_2 . Adopting for the pair distribution function, $f^{(2)}$, the following expansion in a Taylor series about the fixed spatial position \mathbf{r} ,

$$f^{(2)}(\mathbf{c}_1, \mathbf{r}, \mathbf{c}_2, \mathbf{r} + \sigma\mathbf{k}) = f^{(2)}(\mathbf{c}_1, \mathbf{r} - \sigma\mathbf{k}, \mathbf{c}_2, \mathbf{r}) + \sigma k_i \frac{\partial}{\partial r_i} \left(1 - \frac{\sigma}{2!} k_j \frac{\partial}{\partial r_j} + \frac{\sigma^2}{3!} k_j k_m \frac{\partial^2}{\partial r_j \partial r_m} - \dots \right) f^{(2)}(\mathbf{c}_1, \mathbf{r}, \mathbf{c}_2, \mathbf{r} + \sigma\mathbf{k}), \quad (1.44)$$

the expression for $C(\psi)$, computed in details in [Jenkins and Richman, 1985a], is:

$$C(\psi) = \chi(\psi) - \frac{\partial}{\partial r_i} \theta_i(\psi) - \frac{\partial u_j}{\partial r_i} \theta_i \left(\frac{\partial \psi}{\partial C_j} \right). \quad (1.45)$$

We observe that:

$$\chi(\psi) = \frac{1}{2} \int \int \int (\psi'_1 + \psi'_2 - \psi_1 - \psi_2) f^{(2)}(\mathbf{c}_1, \mathbf{r} - \sigma\mathbf{k}, \mathbf{c}_2, \mathbf{r}) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2 \quad (1.46)$$

is the source term,

$$\theta_i(\psi) = -\frac{\sigma}{2} \int \int \int (\psi'_1 - \psi_1) k_i \left(1 - \frac{\sigma}{2!} k_j \frac{\partial}{\partial r_j} + \frac{\sigma^2}{3!} k_j k_m \frac{\partial^2}{\partial r_j \partial r_m} - \dots \right) \times f^{(2)}(\mathbf{c}_1, \mathbf{r}, \mathbf{c}_2, \mathbf{r} + \sigma\mathbf{k}) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2 \quad (1.47)$$

is the flux term, related to the transfer of the generic moment during collisions, while the term $\frac{\partial u_j}{\partial r_i} \theta_i \left(\frac{\partial \psi}{\partial C_j} \right)$ figures only when ψ is a function depending on C . The equation governing the evolution in time of the mean amount, $\langle n\psi \rangle$, is

$$\frac{\partial}{\partial t} \langle n\psi \rangle = n \left\langle \frac{F_i}{m} \frac{\partial \psi}{\partial c_i} \right\rangle - \frac{\partial}{\partial r_i} \langle n c_i \psi \rangle + C(\psi). \quad (1.48)$$

where F_i is the external force acting on a particle. When $\psi = 1$, we recover the conservation law of mass:

$$\frac{D\rho}{Dt} + \rho \frac{\partial u_i}{\partial r_i} = 0, \quad (1.49)$$

where the density $\rho = nm$ and $\frac{D}{Dt} = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial r_i}$ is the time derivative following the mean flow. Inserting the expression of $C(\psi)$, (1.45) and the conservation law (1.49) in (1.48), we obtain:

$$\begin{aligned} \rho \frac{D\langle \psi \rangle}{Dt} + \frac{\partial}{\partial r_i} (\langle \rho C_i \psi \rangle + \theta_i \langle m\psi \rangle) + \rho \left(\frac{D u_i}{Dt} - \frac{F_i}{m} \right) \left\langle \frac{\partial \psi}{\partial C_i} \right\rangle \\ + \left(\left\langle \rho C_i \frac{\partial \psi}{\partial C_j} \right\rangle + \theta_i \left(m \frac{\partial \psi}{\partial C_j} \right) \right) \frac{\partial u_j}{\partial r_i} = \chi \langle m\psi \rangle. \end{aligned} \quad (1.50)$$

From this equation we will determine all the balance laws of the moments. Let us adopt the following notations:

$$M_{i_1, i_2, \dots, i_N} := \langle C_{i_1} C_{i_2} \dots C_{i_N} \rangle \quad (1.51)$$

express the transport of particle properties between collisions;

$$\theta_{j, i_1, i_2, \dots, i_N} := \theta_j \langle m C_{i_1} C_{i_2} \dots C_{i_N} \rangle \quad (1.52)$$

indicate the transfer of particle properties in collisions;

$$\chi_{i_1, i_2, \dots, i_N} := \chi \langle m C_{i_1} C_{i_2} \dots C_{i_N} \rangle \quad (1.53)$$

are the source terms. We note that in the case of diluted gas, particles travel a long distance between them, so when two particles collide, the presence of other nearby particles is ignored and the positions of the two colliding particle centers are not distinct. Furthermore, the phenomenon of transport of the properties of particles during collision prevails over that of transfer and therefore the term (1.52) is neglected. Instead, in the case that we are studying concerning dense gases and granular materials, when two particles collide, their centers are distinct and the transfer term acting on the σ distance between the particle centers can no longer be overlooked. So we will always have to consider in the balance equations the contributions, due to transport M_{i_1, i_2, \dots, i_N} and transfer $\theta_{j, i_1, i_2, \dots, i_N}$. Also we have to take into account the presence of nearby particles during a collision and this is achieved by adopting the pair distribution function:

$$f^{(2)}(\mathbf{c}_1, \mathbf{r}, \mathbf{c}_2, \mathbf{r} + \frac{1}{2}\sigma\mathbf{k}) = g_0 \mathbf{r} + \frac{1}{2}\sigma\mathbf{k} f^{(1)}(\mathbf{c}_1, \mathbf{r}) f^{(1)}(\mathbf{c}_2, \mathbf{r} + \sigma\mathbf{k}), \quad (1.54)$$

where the radial distribution function g_0 , given in (1.8), indicates the likelihood of a collision. If we set $\psi = C_i$ in (1.50), we obtain the balance law of linear momentum,

$$\rho \frac{Du_i}{Dt} + \frac{\partial}{\partial r_j} (\rho M_{ij} + \theta_{ij}) = nF_i, \quad (1.55)$$

where M_{ij} is the transport term, θ_{ij} the transfer term and the sum $P_{ij} = \rho M_{ij} + \theta_{ij}$ is the pressure tensor. If we take $\psi = C^2$ with the temperature $T = \frac{\langle C^2 \rangle}{3}$, we recover the balance law of energy,

$$\frac{3}{2} \rho \frac{DT}{Dt} + \frac{1}{2} \frac{\partial}{\partial r_i} (\rho M_{ijj} + \theta_{ijj}) + P_{ij} \frac{\partial u_j}{\partial r_i} = \frac{1}{2} \chi_{jj}, \quad (1.56)$$

in which ρM_{ijj} is the transport term, θ_{ijj} the transfer term, the sum $q_i = \rho M_{ijj} + \theta_{ijj}$ is the heat flux and $\frac{1}{2} \chi_{jj}$ the dissipation of energy because collisions are inelastic. If we set $\psi = C_i C_j$ and use the energy law, we obtain the balance law for the deviatoric part, \hat{M}_{ij} of the second moment of velocity, M_{ij} ,

$$\frac{1}{2} \rho \dot{\hat{M}}_{ij} + \left(Q_{kij} - \frac{1}{3} Q_k \delta_{ij} \right)_{,k} + \left(P_{k(i} u_{j),k} - \frac{1}{3} P_{kn} u_{n,k} \delta_{ij} \right) = \frac{1}{2} \hat{\chi}_{ij}, \quad (1.57)$$

where the overdot stands for the time derivative, the comma the differentiation with respect to position, $Q_{kij} := \frac{(\rho M_{kij} + \theta_{kij})}{2}$ and $\hat{\chi}_{ij} = \chi_{ij} - \chi_{kk} \frac{\delta_{ij}}{3}$. If we take $\psi = C_i C_j C_k$, we determine the balance law for the third moment of velocity,

$$\rho \dot{M}_{ijk} + 2Q_{nij,k} - 3M_{(ij} P_{k)n,n} + 6Q_{n(ij} u_{k),n} = \chi_{ijk}, \quad (1.58)$$

where $Q_{nij} = \frac{1}{2} (\rho M_{nij} + \theta_{nij})$. In order to solve the set of balance laws, we approximate the single particle distribution function to the infinite series as Grad made in [Grad, 1958]:

$$f^{(1)}(\mathbf{c}, \mathbf{r}, t) = \left(1 - a_i \frac{\partial}{\partial c_i} + \frac{a_{ij}}{2!} \frac{\partial^2}{\partial c_i \partial c_j} - \frac{a_{ijk}}{3!} \frac{\partial^3}{\partial c_i \partial c_j \partial c_k} + \dots \right) f_0^{(1)}(\mathbf{c}, \mathbf{r}, t) \quad (1.59)$$

where

$$f_0^{(1)}(\mathbf{c}, \mathbf{r}, t) = \frac{n}{(2\pi T)^{3/2}} \exp\left(-\frac{c^2}{2T}\right) \quad (1.60)$$

is the Maxwellian distribution and the coefficients $a_i, a_{ij}, a_{ijk}, \dots$, are the first, second, third order tensors, depending on \mathbf{r} and t and symmetric in all of their indices. We observe that $a_i = 0$ in order to vanish the mean of the relative velocity, C and $a_{ii} = 0$ because of the definition of the temperature. Following [Jenkins and Richman, 1985a], we recover from (1.59) the expressions for the mean value of the generic moment (1.51) as

$$M_{i_1, i_2, \dots, i_N} = N! \sum_{p=0}^N \frac{1}{p!(N-p)!} a_{(i_1 \dots i_p} \langle C_{i_{p+1}} \dots C_{i_N} \rangle^0, \quad (1.61)$$

where

$$\langle C_{i_{p+1}} \dots C_{i_N} \rangle^0 := \frac{1}{n} \int C_{i_{p+1}} \dots C_{i_N} f_0^{(1)}(\mathbf{c}, \mathbf{r}, t) d\mathbf{c} \quad (1.62)$$

is the Maxwellian mean of $C_{i_{p+1}} \dots C_{i_N}$. So, we determine:

$$M_{ij} = T\delta_{ij} + a_{ij}, \quad (1.63)$$

$$M_{ijk} = a_{ijk}, \quad (1.64)$$

and

$$M_{ijkp} = 3T^2\delta_{(ij}\delta_{kp)} + 6Ta_{(ij}\delta_{kp)} + a_{ijkp}. \quad (1.65)$$

The expressions of the pair distribution function (1.54) and the single velocity distribution function (1.59) allow to find the source terms (1.46) and the flux terms (1.47), but it is necessary to truncate (1.59) at the N term a_{i_1, i_2, \dots, i_N} to have a finite number of unknowns $\rho, u_i, T, \dots, a_{i_1, i_2, \dots, i_N}$, determined by the system of N balance equations. Grad [Grad, 1958] truncated the single velocity distribution function to the third order. An alternative method is that of Maxwellian iterations, which Truesdell and Muncaster [Truesdell and Muncaster, 1980] worked out for diluted gases and which Jenkins and Richman [Jenkins and Richman, 1985a] extended to dense gases.

We truncate the single particle distribution function (1.59) after its first three terms, so the unknown variables are ρ, u_i, T, a_{ij} and a_{ijk} . The last term has no direct physical meaning but it is related to the heat flux a_{iil} . So we adopt the decomposition of a_{ijk} into deviatoric and isotropic parts:

$$a_{ijk} = \alpha_{ijk} + \frac{1}{5}(a_{iil}\delta_{jk} + a_{jll}\delta_{ik} + a_{kll}\delta_{ij}) \quad (1.66)$$

and suppose that the deviatoric part α_{ijk} vanishes. Definitely, we have 13 moments for a set of thirteen balance equations: the conservation law for mass, the balance law of momentum, the balance law of energy, the balance of the second moment and the balance of the third moment. Here we determine the last two balance laws. Using (1.63), (1.64) and (1.66), the balance law for the second moment (1.57) assumes the form

$$\begin{aligned} & \rho \frac{Da_{ij}}{Dt} + \frac{1}{5} \left(\frac{\partial(\rho a_{ikk})}{\partial r_j} + \frac{\partial(\rho a_{jkk})}{\partial r_i} - \frac{2}{3} \frac{\partial(\rho a_{pkk})}{\partial r_p} \delta_{ij} \right) + 2\rho T \hat{D}_{ij} \\ & + \left((\rho a_{ki} + \theta_{ki}) \frac{\partial u_j}{\partial r_k} + (\rho a_{kj} + \theta_{kj}) \frac{\partial u_i}{\partial r_k} - \frac{2}{3} (\rho a_{kp} + \theta_{kp}) \frac{\partial u_p}{\partial r_k} \delta_{ij} \right) \\ & + \frac{\partial}{\partial r_k} (\theta_{kij} - \frac{1}{3} \theta_{kpp} \delta_{ij}) = \chi_{ij} - \frac{1}{3} \chi_{kk} \delta_{ij}, \end{aligned} \quad (1.67)$$

where \hat{D}_{ij} is the deviatoric part of the strain tensor $D_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$. The balance law for the third moment (1.58), setting $j = k$ and using (1.65) with $a_{ijkp} = 0$, becomes:

$$\begin{aligned} & \rho \frac{Da_{ikk}}{Dt} + 5 \frac{\partial(\rho T^2)}{\partial r_i} + 7 \frac{\partial(\rho T a_{ij})}{\partial r_j} + \frac{\partial}{\partial r_n} \theta_{nijj} - (5T\delta_{ij} + 2a_{ij}) \frac{\partial}{\partial r_k} (\rho T \delta_{jk} + \rho a_{jk} + \theta_{jk}) \\ & + \frac{\rho}{5} \left(7a_{jkk} \frac{\partial u_i}{\partial r_j} + 2a_{jkk} \frac{\partial u_j}{\partial r_i} + 2a_{ikk} \frac{\partial u_j}{\partial r_j} \right) + 2\theta_{kij} \frac{\partial u_j}{\partial r_k} + \theta_{kjj} \frac{\partial u_i}{\partial r_k} = \chi_{ijj}. \end{aligned} \quad (1.68)$$

In the case of dense gases, the positions of the centers of two colliding particles are distinct. This means that in the expression of the pair distribution function (1.54), the functions of the velocity distributions of the two particles are evaluated at different points in space. To make source and flux terms dependent on unknown fields,

evaluated at the same point, approximations with series and truncations must be adopted. In addition, gradients of unknown fields should be assumed to be of a small order of magnitude.

1.3.2 Production terms

Based on the assumption that the gradients of the main fields are small, we approach the pair distribution function with Taylor series that will allow us to determine the source term and flux term of each balance equation. Using the Taylor series expansion

$$f^{(2)}(\mathbf{c}_1, \mathbf{r} - \sigma \mathbf{k}, \mathbf{c}_2, \mathbf{r}) = g_0(\mathbf{r}) \left(f^{(1)}(\mathbf{c}_1, \mathbf{r}) - \sigma k_i \frac{\partial f^{(1)}(\mathbf{c}_1, \mathbf{r})}{\partial r_i} \right) f^{(1)}(\mathbf{c}_2, \mathbf{r}) - \frac{\sigma}{2} k_i \frac{\partial g_0(\mathbf{r})}{\partial r_i} f^{(1)}(\mathbf{c}_1, \mathbf{r}) f^{(1)}(\mathbf{c}_2, \mathbf{r}), \quad (1.69)$$

in (1.46), we recover

$$\chi(\varphi) = \frac{g_0(\mathbf{x})}{2} \int \int \int (\psi'_1 + \psi'_2 - \psi_1 - \psi_2) f^{(1)}(\mathbf{c}_1, \mathbf{r}) f^{(1)}(\mathbf{c}_2, \mathbf{r}) \times \left[1 + \frac{\sigma}{2} k_i \frac{\partial}{\partial r_i} \ln \frac{f^{(1)}(\mathbf{c}_2, \mathbf{r})}{f^{(1)}(\mathbf{c}_1, \mathbf{r})} \right] \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2. \quad (1.70)$$

Employing

$$f^{(2)}(\mathbf{c}_1, \mathbf{r}, \mathbf{c}_2, \mathbf{r} + \sigma \mathbf{k}) = g_0(\mathbf{r}) \left(f^{(1)}(\mathbf{c}_2, \mathbf{r}) + \sigma k_i \frac{\partial f^{(1)}(\mathbf{c}_2, \mathbf{r})}{\partial r_i} \right) f^{(1)}(\mathbf{c}_1, \mathbf{r}) + \frac{\sigma}{2} k_i \frac{\partial g_0(\mathbf{r})}{\partial r_i} f^{(1)}(\mathbf{c}_1, \mathbf{r}) f^{(1)}(\mathbf{c}_2, \mathbf{r}), \quad (1.71)$$

into (1.47), we obtain

$$\theta_i(\varphi) = -\sigma \frac{g_0(\mathbf{x})}{2} \int \int \int (\psi'_1 - \psi_1) k_i f^{(1)}(\mathbf{c}_1, \mathbf{r}) f^{(1)}(\mathbf{c}_2, \mathbf{r}) \times \left[1 + \frac{\sigma}{2} k_j \frac{\partial}{\partial r_j} \left(\ln \frac{f^{(1)}(\mathbf{c}_2, \mathbf{r})}{f^{(1)}(\mathbf{c}_1, \mathbf{r})} \right) \right] \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2. \quad (1.72)$$

Jenkins and Richman [Jenkins and Richman, 1985a] provide simplified expressions for flux and source terms, which are linear in velocity and temperature gradients. In fact quadratic terms of the moments a_{ij} and a_{ijk} or the products of these moments for the gradients of the main fields are neglected. The approximate expressions of the flux and source are respectively:

$$\begin{aligned} \theta_i(\psi) &= A_i(\psi) + B_i(\psi) + a_{jk} B_{ijk}(\psi) + a_{jkp} B_{ijkp}(\psi) \\ \chi(\psi) &= E(\psi) + F(\psi) + a_{jk} F_{jk}(\psi) + a_{ijk} F_{ijk}(\psi) \end{aligned} \quad (1.73)$$

where the integrals are given by

$$\begin{aligned}
A_i(\psi) &= -\frac{\sigma}{2} g_0 \int \int \int (\psi'_1 - \psi_1) k_i f_{01} f_{02} \sigma^2 (\mathbf{g} \cdot \mathbf{k}) \, d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2, \\
B_i(\psi) &= -\frac{\sigma^2}{4} g_0 \int \int \int (\psi'_1 - \psi_1) k_i k_m f_{01} f_{02} \frac{\partial}{\partial r_m} \left(\ln \frac{f_{02}}{f_{01}} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) \, d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2, \\
B_{ijk}(\psi) &= -\frac{\sigma}{4} g_0 \int \int \int (\psi'_1 - \psi_1) k_i \left(f_{01} \frac{\partial^2 f_{02}}{\partial c_{2j} \partial c_{2k}} + f_{02} \frac{\partial^2 f_{01}}{\partial c_{1j} \partial c_{1k}} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) \, d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2, \\
B_{ijkp}(\psi) &= \frac{\sigma g_0}{12} \int \int \int (\psi'_1 - \psi_1) k_i \left(f_{01} \frac{\partial^3 f_{02}}{\partial c_{2j} \partial c_{2k} \partial c_{2p}} + f_{02} \frac{\partial^3 f_{01}}{\partial c_{1j} \partial c_{1k} \partial c_{1p}} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) \, d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2.
\end{aligned} \tag{1.74}$$

and

$$\begin{aligned}
E(\psi) &= \frac{g_0}{2} \int \int \int \Delta(\psi) f_{01} f_{02} \sigma^2 (\mathbf{g} \cdot \mathbf{k}) \, d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2, \\
F(\psi) &= \sigma \frac{g_0}{4} \int \int \int \Delta(\psi) k_m f_{01} f_{02} \frac{\partial}{\partial r_m} \left(\ln \frac{f_{02}}{f_{01}} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) \, d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2, \\
F_{ij}(\psi) &= \frac{g_0}{4} \int \int \int \Delta(\psi) \left(f_{01} \frac{\partial^2 f_{02}}{\partial c_{2i} \partial c_{2j}} + f_{02} \frac{\partial^2 f_{01}}{\partial c_{1i} \partial c_{1j}} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) \, d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2, \\
F_{ijk}(\psi) &= -\frac{g_0}{12} \int \int \int \Delta(\psi) \left(f_{01} \frac{\partial^3 f_{02}}{\partial c_{2i} \partial c_{2j} \partial c_{2k}} + f_{02} \frac{\partial^3 f_{01}}{\partial c_{1i} \partial c_{1j} \partial c_{1k}} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) \, d\mathbf{k} d\mathbf{c}_1 d\mathbf{c}_2.
\end{aligned} \tag{1.75}$$

with $\Delta = \psi'_1 + \psi'_2 - \psi_1 - \psi_2$, $f_{01} = f_0^{(1)}(c_1, \mathbf{r})$ and $f_{02} = f_0^{(1)}(c_2, \mathbf{r})$. The use of (1.73) instead of (1.46) and (1.47) allows us to determine with a good degree of approximation the values of the source and flux terms. The computations involve using velocity change formulas (1.3). During this dissertation we will try to deal with the results of Jenkins and Richman [Jenkins and Richman, 1985a] in the context of Extended Thermodynamics and to extend them to the 14-moment system for dense gases.

1.3.3 Approximation of Moments

In order to evaluate the time derivatives of a_{ij} and a_{ill} , we consider the simple case in which the main fields ρ , u_i and T are constants and a_{ij} and a_{ill} depend only on time. In this way (1.67) and (1.68) provide:

$$\dot{a}_{ij} + \frac{1}{\bar{\tau}} = 0, \tag{1.76}$$

and

$$\dot{a}_{ikk} + \frac{1}{\hat{\tau}} = 0, \tag{1.77}$$

where $\bar{\tau}$ and $\hat{\tau}$ are relaxation times, proportional to

$$\frac{1}{\nu g_0} \frac{\sigma U}{L T_0^{\frac{1}{2}}}. \tag{1.78}$$

We observe that when $\nu \in]0.2, 0.6[$, then $\nu g_0 \in]0.4, 5[$ for the expression (1.8). In this range, relaxation times are small if the parameter $\frac{\sigma U}{L T_0^{\frac{1}{2}}}$ is small. As a consequence time derivative of a_{ij} and a_{ill} are neglected. We assume in what follows that the dimensionless parameters

$$\frac{\sigma}{L}, \frac{a_{ij}}{T_0}, \frac{a_{ijk}}{T_0^{\frac{3}{2}}}, \frac{\sigma U}{L T_0^{\frac{1}{2}}} \tag{1.79}$$

are small. Solving the dimensionless form of (1.67), we determine the second moment:

$$\rho a_{ij} = -2\bar{\mu}\hat{D}_{ij} \quad (1.80)$$

where

$$\bar{\mu} = \alpha \left(1 + \frac{2}{5}v g_0(3e - 1)(1 + e) \right) \quad (1.81)$$

is the transport shear viscosity, with

$$2\alpha = \frac{5mT^{\frac{1}{2}}}{2\sigma^2 g_0(1 + e)(3 - e)\pi^{\frac{1}{2}}}. \quad (1.82)$$

Considering the dimensionless form of (1.68), we obtain:

$$\frac{1}{2}\rho a_{ikk} = -\bar{\varepsilon}\frac{\partial T}{\partial r_i} + \bar{\delta}\frac{\partial \rho}{\partial r_i} \quad (1.83)$$

where

$$\bar{\varepsilon} = \beta \left(1 + \frac{3}{5}v g_0(1 + e)^2(2e - 1) \right) \quad (1.84)$$

is the transport coefficient, analogous to the thermal conductivity for dilute gas, with

$$\beta = \frac{75mT^{\frac{1}{2}}}{2\sigma^2 g_0(1 + e)(49 - 33e)\pi^{\frac{1}{2}}} \quad (1.85)$$

and

$$\bar{\delta} = \frac{15e(1 - e)\pi^{\frac{1}{2}}\sigma T^{\frac{3}{2}}}{4(49 - 33e)v g_0} \frac{d(v^2 g_0)}{dv} \quad (1.86)$$

that is the transport coefficient, related to the density gradient. Employing (1.73) together with (1.74) and (1.75), we are able to determine respectively the transfer part of the pressure tensor and heat flux and the dissipation of energy:

$$\theta_{ij} = [\rho T(2v g_0(1 + e)) - \omega D_{kk}] - \left[2\bar{\mu} \left(\frac{4}{5}v g_0(1 + e) \right) + \frac{6}{5}\omega \right] \hat{D}_{ij}, \quad (1.87)$$

where

$$\omega = \frac{8mv^2 g_0(1 + e)T^{\frac{1}{2}}}{\pi^{\frac{3}{2}}\sigma^2} \quad (1.88)$$

is the bulk viscosity,

$$\frac{1}{2}\theta_{ikk} = - \left[\bar{\varepsilon} \left(\frac{6v g_0(1 + e)}{5} \right) + \frac{3\omega}{2} \right] + \bar{\delta} \left(\frac{6v g_0(1 + e)}{5} \right) \frac{\partial \rho}{\partial r_i}, \quad (1.89)$$

$$\gamma = \frac{3\omega(1 - e)}{4\sigma^2} (12T - 3\pi^{\frac{3}{2}}\sigma T^{\frac{1}{2}} D_{ii}). \quad (1.90)$$

Finally the total expression of the pressure tensor is

$$P_{ij} = (p - \omega D_{kk})\delta_{ij} - 2\mu\hat{D}_{ij}, \quad (1.91)$$

where

$$p = \rho T(1 + 2v g_0(1 + e)) \quad (1.92)$$

is the pressure and

$$\mu = \bar{\mu} \left(1 + \frac{4}{5} \nu g_0 (1 + e) \right) + \frac{3}{5} \omega \quad (1.93)$$

is the shear viscosity. The total energy flux can be expressed as

$$Q_i = -\varkappa \frac{\partial T}{\partial r_i} + \delta \frac{\partial \rho}{\partial r_i} \quad (1.94)$$

where

$$\varkappa = \bar{\varkappa} \left(1 + \frac{6}{5} \nu g_0 (1 + e) \right) \frac{3}{2} \omega, \quad (1.95)$$

$$\delta = \bar{\delta} \left(1 + \frac{6}{5} \nu g_0 (1 + e) \right). \quad (1.96)$$

To verify that the approximation made is physically acceptable, we study a stationary flow between two parallel plates, which move relative to each other. The density and temperature are constant, while the velocity varies linearly with the distance between the plates. Applying these hypotheses to the energy balance equation (1.56) and using the formulas for the pressure tensor (1.91) and the energy dissipation rate (1.90), we arrive at the relations:

$$\left(\frac{\sigma U}{LT^{\frac{1}{2}}} \right)^2 = \frac{9\omega}{2\mu} (1 - e), \quad (1.97)$$

where the term to first member is considered small in the approximation. Observing that for values of $\nu \in]0.3, 0.6[$, the ratio between ω and μ varies in the range $]0.5, 2[$, it follows that the coefficient $(1 - e)$ must be small to make the term to first member is small. This implies that we must neglect the terms that in the constitutive relations contain $\bar{\delta}$, proportional to $(1 - e)$ together with the term D_{ii} in the expression of the rate of energy dissipation (1.90). So the constitutive relations become

$$P_{ij} = (p - \omega D_{kk}) \delta_{ij} - 2\mu \hat{D}_{ij} \quad (1.98)$$

$$Q_i = -\varkappa \frac{\partial T}{\partial r_i}, \quad (1.99)$$

$$\gamma = \frac{9\omega(1 - e)T}{\sigma^2}. \quad (1.100)$$

These relations are experimentally valid because they are in agreement with data obtained by Lun in the work Lun et al., 1984.

1.4 Concluding remarks

In this chapter we have presented the results of [Jenkins and Savage, 1983] and [Jenkins and Richman, 1985a]. In the work [Jenkins and Savage, 1983], using the Maxwell equation, the balance laws for mass, momentum and energy are derived. The two authors then approximate the distribution function $f^{(2)}(c_1, r_1, c_2, r_2, t)$ that expresses the collisions between two particles as the product of the velocity distribution function of each particle $f^{(1)}(c_i, r_i)$, regarded as the Maxwellian function, and the radial distribution function $g(r_1, r_2)$. By developing Taylor's first-order series of the function $f^{(2)}(c_1, r_1, c_2, r_2, t)$, they determine the constitutive relations for the pressure tensor P_{ij} , the heat flux q_i and the energy dissipation γ . In the paper [Jenkins

and Richman, 1985a] in addition to the balance laws for mass, momentum and energy, the balance laws for stress tensors and heat flux are also derived. Adopting a Taylor series development for the velocity distribution function of each single particle $f^{(1)}$, the parts M_{ij} and M_{ill} of the pressure tensor P_{ij} and heat flux q_i , due to the transport of momentum and energy between collisions respectively, are determined. Instead the use of the formulas (1.73) allows to compute the parts θ_{ij} and θ_{ill} of the pressure tensor and heat flux and the energy dissipation γ , due to the transfer of momentum and energy during collisions. We'll use the formulas 1.73 in Chapter 3 to determine all the production terms for a fourteen moments model.

Chapter 2

An Extended Thermodynamic Model of 13 moments for granular gas

2.1 Introduction

Many works in the literature have been devoted to rarefied gases, characterized by elastic collisions, especially in the field of kinetic theory. The 13-moment Grad method is an example. The aim of this chapter is to extend the treatment to other gases, whose molecules are involved in inelastic collisions. The inelasticity implies that the total energy is not conserved, but part of it turns into heat, and that means a decay of the gas temperature.

In the previous chapter we presented in detail some works by Jenkins and Richman on kinetic models for dense gases. Mention should also be made of Kremer and Marques [Kremer and Marques Jr, 2011] contribution to a 14-moment theory for dilute granular gases, adding to the thirteen moments of mass density, velocity, stress tensor, and heat flow, a fourth-order scalar moment. They determined spatially homogeneous solutions that reveal the temporal decay of temperature, stress tensor, heat flow and scalar moment of order 4. Moreover, they showed that the time decay of the temperature is very close to that predicted by Haff's law [Brilliantov and Pöschel, 2004; Haff, 1983]. Kremer and Marques also study the dynamic behavior of small local perturbations from spatially homogeneous solutions due to spontaneous internal fluctuations by considering a thirteen field theory. The study of the stability of longitudinal and transverse waves in dilute inelastic gases was extended to more moments in [Gupta, Shukla, and Torrilhon, 2018b], where the authors found unstable longitudinal and transverse modes and compared their results with other existing theories (see [Gupta, Shukla, and Torrilhon, 2018b] and the references therein). In this Chapter we aim to investigate the behavior of granular gas in the context of Extended Thermodynamics and to derive a quasi linear system of differential equations for 13 moments. The model has to be closed by constitutive relations that are determined by invoking universal physical principles, such as the entropic inequality, the convexity of entropy and the principle of Galilean invariance. We integrate the system in the linear case and determine in one dimensional space the spatially homogeneous solutions and the stationary solutions. We verify that the solutions are acceptable and compatible with the hyperbolicity region of the model and with the region in which the residual inequality of entropy is non-negative.

2.2 Derivation of the field equations in Extended Thermodynamics

For the description of the behavior of granular gas we introduce the field variables: the density $\rho(t, \mathbf{x})$, the velocity $v_i(t, \mathbf{x})$, the temperature $T(t, \mathbf{x})$, the deviatoric part of the stress tensor $\rho_{\langle ij \rangle}(t, \mathbf{x})$ and the heat flux $q_i(t, \mathbf{x})$. In order to obtain these 13 fields, we assume as 13 field equations the balance equations for mass, momentum, momentum flux and energy, as follows

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} &= 0, \\ \frac{\partial \rho v_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} &= \rho f_i, \\ \frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} &= 2\rho v_{(i} f_{j)} + P_{ij}, \\ \frac{\partial F_{ill}}{\partial t} + \frac{\partial F_{ikl}}{\partial x_k} &= 3F_{(il} f_{l)} + P_{ill}. \end{aligned} \tag{2.1}$$

In these equations f_i is the specific external body force and round brackets indicate symmetrization. The set of balance equations (2.1) is the classical hierarchy of 13 equations for classical monatomic gases [Müller and Ruggeri, 2013]. The fluxes in every equations are the densities of the following equations. P_{ij} and P_{ill} represent the production terms. We assume here to be in presence of dilute gases of inelastic spheres, so we follow the results of Jenkins and Richman [Jenkins and Richman, 1985a] in order to evaluate production terms.

This system of field equations is not closed, since there are unknown quantities that are not expressed explicitly in terms of the fields. In order to close it, we need to express the quantities in (2.1), as known functions of the fields in a form that depends on the material under consideration, called constitutive quantities. In this chapter we follow the methods of Rational Extended Thermodynamics [Müller and Ruggeri, 2013] in order to derive the constitutive functions.

2.2.1 Galilean invariance

We require that the balance equations (2.1) hold in every inertial frame, so these equations must be invariant under a Galilean transformation. This requirement enables us to determine the velocity dependence of the quantities in (2.1) on the velocity field [Müller and Ruggeri, 2013]. In particular the following decomposition must hold

$$\begin{aligned} F_{ij} &= \rho_{ij} + \rho v_i v_j, \\ F_{ijk} &= \rho_{ijk} + 3\rho_{(ij} v_{k)} + \rho v_i v_j v_k, \\ F_{ikll} &= \rho_{ikll} + 4\rho_{(ikl} v_{l)} + 6\rho_{(ik} v_l v_{l)} + \rho v^2 v_i v_k, \end{aligned} \tag{2.2}$$

where the moments $\rho_{i_1, i_2, \dots, i_N}$ do not depend on the velocity field. They are called for this reason internal moments. Some of them can be identify with common thermodynamic variables, indeed $\rho_{ij} = -t_{ij}$, where t_{ij} is the stress tensor, and $\rho_{ill} = 2q_i$ with q_i the heat flux. For the production terms the following decomposition must be valid

$$\begin{aligned} P_{ij} &= \psi_{ij}, \\ P_{ill} &= \psi_{ill} + 3\psi_{(il} v_{l)}, \end{aligned} \tag{2.3}$$

with ψ_{ij} and ψ_{ill} independent on the velocity field.

By substitution of (2.2) and (4.5) into the balance equations (2.1), one obtains a more compact form of the equations, that is

$$\begin{aligned}
\frac{d\rho}{dt} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\
\rho \frac{dv_i}{dt} + \frac{\partial \rho_{ik}}{\partial x_k} &= \rho f_i, \\
\frac{d\rho_{ij}}{dt} + \frac{\partial \rho_{ijk}}{\partial x_k} + \rho_{ij} \frac{\partial v_k}{\partial x_k} + 2\rho_{k(i} \frac{\partial v_{j)}}{\partial x_k} &= \psi_{ij}, \\
\frac{d\rho_{ill}}{dt} + \frac{\partial \rho_{ikll}}{\partial x_k} + \rho_{ill} \frac{\partial v_k}{\partial x_k} + 3\rho_{k(il} \frac{\partial v_l)}{\partial x_k} - 3\frac{\rho_{(il}}{\rho} \frac{\partial \rho_{l)k}}{\partial x_k} &= \psi_{ill}.
\end{aligned} \tag{2.4}$$

The first two equations represent the conservation laws of mass and momentum. The trace of the third equation represents the balance law of energy. In fact for monatomic gases the internal energy ρu is given by $\rho u = \frac{1}{2}\rho_{ll} = \frac{3}{2}\rho\theta$ with θ the so-called granular temperature.

Equations (2.4) represent 13 equations for the 13 fields ρ , v_i , θ , $\rho_{\langle ij \rangle}$ and q_k . Unfortunately, these equations are not closed for the occurrence of the constitutive quantities $\rho_{\langle ijk \rangle}$, ρ_{ikll} , ψ_{ij} and ψ_{ill} . Following the guidelines of Rational Extended Thermodynamics [Müller and Ruggeri, 2013], we assume that these quantities depend locally on the fields, that is they depend only on the fields and not on their derivatives, i.e.

$$\begin{aligned}
\rho_{\langle ijk \rangle} &= \rho_{\langle ijk \rangle}(\rho, \theta, \rho_{\langle sr \rangle}, q_m), \\
\rho_{ikll} &= \rho_{ikll}(\rho, \theta, \rho_{\langle sr \rangle}, q_m), \\
\psi_{ij} &= \psi_{ij}(\rho, \theta, \rho_{\langle sr \rangle}, q_m), \\
\psi_{ill} &= \psi_{ill}(\rho, \theta, \rho_{\langle sr \rangle}, q_m).
\end{aligned} \tag{2.5}$$

In the next chapter, we restrict their generality, using the entropy principle.

2.2.2 Entropy principle

The entropy principle asserts the existence of a concave entropy density h , an entropy flux h_k and an entropy production Σ , such that the balance law

$$\frac{\partial h}{\partial t} + \frac{\partial h_k}{\partial x_k} = \Sigma \geq 0 \tag{2.6}$$

is valid for all thermodynamic process, that is for all solutions of the field equations (2.4). Therefore equations (2.4) can be considered as constrains for the validity of the entropy principle. Following the methods of Rational Extended Thermodynamics, we take into account theses constrains by introducing the so-called Lagrange Multipliers λ , [Liu, 1972]. In this way the following relation

$$\begin{aligned}
&\frac{\partial h}{\partial t} + \frac{\partial h_k}{\partial x_k} + \\
&-\lambda \left[\frac{d\rho}{dt} + \rho \frac{\partial v_k}{\partial x_k} \right] + \\
&-\lambda_i \left[\rho \frac{dv_i}{dt} + \frac{\partial \rho_{ik}}{\partial x_k} - \rho f_i \right] + \\
&-\lambda_{ij} \left[\frac{d\rho_{ij}}{dt} + \frac{\partial \rho_{ijk}}{\partial x_k} + \rho_{ij} \frac{\partial v_k}{\partial x_k} + 2\rho_{k(i} \frac{\partial v_{j)}}{\partial x_k} - \psi_{ij} \right] + \\
&-\lambda_{ill} \left[\frac{d\rho_{ill}}{dt} + \frac{\partial \rho_{ikll}}{\partial x_k} + \rho_{ill} \frac{\partial v_k}{\partial x_k} + 3\rho_{k(il} \frac{\partial v_l)}{\partial x_k} - 3\frac{\rho_{(il}}{\rho} \frac{\partial \rho_{l)k}}{\partial x_k} - \psi_{ill} \right] = \Sigma \geq 0
\end{aligned} \tag{2.7}$$

must be valid for all fields $\rho, v_i, \theta, \rho_{\langle ij \rangle}$ and q_i .

For the exploitation of relation (2.7), the entropy quantities and the Lagrange multipliers must be expressed as functions of the fields. In particular the entropy flux, with the requirement of Galileian invariance, becomes

$$h_k = hv_k + \phi_k \quad (2.8)$$

with

$$\begin{aligned} h &= h(\rho, \theta, \rho_{\langle sr \rangle}, q_m), \\ \phi_k &= \phi_k(\rho, \theta, \rho_{\langle sr \rangle}, q_m) \end{aligned} \quad (2.9)$$

and the same dependence holds for the Lagrange multipliers λ .

Since we are interested in processes not far from the equilibrium state, characterized by vanishing fluxes $\rho_{\langle ik \rangle}$ and q_i , we expand the constitutive functions in the neighborhood of the equilibrium obtaining for the entropy quantities and the Lagrange multipliers the following expressions

$$\begin{aligned} h &= h_0 + h_1 \rho_{\langle ij \rangle} \rho_{\langle ij \rangle} + h_2 q_i q_i, \\ \phi_k &= \phi_1 q_k + \phi_2 \rho_{\langle lk \rangle} q_l, \\ \lambda &= \lambda_0 + \lambda_1 \rho_{\langle ij \rangle} \rho_{\langle ij \rangle} + \lambda_2 q_l q_l, \\ \lambda_i &= \omega_1 q_i + \omega_2 \rho_{\langle il \rangle} q_l, \\ \lambda_{ij} &= \nu_0 \delta_{ij} + \nu_1 \rho_{\langle ij \rangle} + \nu_2 \rho_{\langle il \rangle} \rho_{\langle lj \rangle} + \nu_3 q_i q_j, \\ \lambda_{ill} &= \sigma_1 q_i + \sigma_2 \rho_{\langle il \rangle} q_l \end{aligned} \quad (2.10)$$

and

$$\begin{aligned} \rho_{ijk} &= \frac{2}{5} q_i \delta_{jk}, \\ \rho_{ijll} &= \gamma_0 \delta_{ij} + \gamma_1 \rho_{\langle ij \rangle} \end{aligned} \quad (2.11)$$

for the constitutive equations.

All functions in (2.10) and (2.11) depend only on the equilibrium variables that are (ρ, θ) .

Substituting (2.10) and (2.11) into the entropy inequality (2.7) implies an equality that must be satisfied for all fields $(\rho, \theta, \rho_{\langle sr \rangle}, q_m)$. Therefore, setting the coefficients of the derivatives of $(\rho, \theta, \rho_{\langle sr \rangle}, q_m)$ equal to zero, one gets a set of equations for the determination of the functions in (2.10) and (2.11).

At equilibrium we have

$$\frac{\partial h_0}{\partial \rho} = \lambda_0 \quad \text{and} \quad \frac{\partial h_0}{\partial \rho u} = 2\nu_0, \quad (2.12)$$

so for dh_0 we have

$$dh_0 = \lambda_0 d\rho + \nu_0 d\rho_{ll} = \lambda_0 d\rho + 2\nu_0 d[\rho u] \quad (2.13)$$

with u the specific internal energy. By comparison of this relation with the Gibbs equation we can identify the equilibrium values of the Lagrange multipliers, i.e. we get

$$\nu_0 = \frac{1}{2\theta} \quad \text{and} \quad \lambda_0 = -\frac{g}{\theta}, \quad (2.14)$$

where $g = u - \theta \frac{h_0}{\rho} + \frac{p}{\rho}$ is the specific free enthalpy or Gibbs free energy.

After some long but simple calculations, the remaining fields become

$$\begin{aligned}
h &= h_0(\rho, \theta) - \frac{1}{4\rho\theta^2}\rho_{\langle ij \rangle}\rho_{\langle ij \rangle} - \frac{1}{5\rho^2\theta^3}q_i q_i, \\
\phi_k &= \frac{1}{\theta}q_k - \frac{2}{5\rho\theta^2}\rho_{\langle lk \rangle}q_l, \\
\lambda &= -\frac{g}{\theta} - \frac{1}{4\rho^2\theta^2}\rho_{\langle ij \rangle}\rho_{\langle ij \rangle} - \frac{2}{5\rho^2\theta^5}q_l q_l, \\
\lambda_i &= 0, \\
\lambda_{ij} &= \frac{1}{2\theta}\delta_{ij} - \frac{1}{2\rho\theta^2}\rho_{\langle ij \rangle} + \frac{1}{2\rho^2\theta^3}\rho_{\langle il \rangle}\rho_{\langle lj \rangle} + \frac{3}{5\rho^2\theta^4}q_i q_j, \\
\lambda_{ill} &= -\frac{1}{5\rho\theta^3}q_i + \frac{9}{25\rho^2\theta^4}\rho_{\langle il \rangle}q_l,
\end{aligned} \tag{2.15}$$

with the linear constitutive functions

$$\begin{aligned}
\rho_{ijk} &= \frac{6}{5}q_i\delta_{jk}, \\
\rho_{ijll} &= 5\rho\theta^2\delta_{ij} + 7\theta\rho_{\langle ij \rangle}.
\end{aligned} \tag{2.16}$$

So we have closed the system since the constitutive functions for the variables ρ_{ijk} and ρ_{ijll} are explicitly determined in terms of the unknown fields.

In order to verify completely the balance of entropy, it remains to satisfy the convexity of entropy density h and to prove the residual inequality

$$\Sigma = \lambda_{ij}\psi_{ij} + \lambda_{ill}\psi_{ill} \geq 0, \tag{2.17}$$

that will be done in the next chapter when the production terms will be determined.

2.2.3 Convexity region

We prove here that the entropy density (4.9)₁ is a convex function, at least near the equilibrium state. First of all, we require that the Hessian matrix of h_0 is positive-defined with respect to the variables ρ and ρ_{ll} . Using the relations (2.12), obtained from the Gibbs equation, we get

$$\begin{vmatrix} -\left(\frac{\partial^2 h_0}{\partial \rho^2}\right)_{\rho_{ll}} & -\frac{\partial^2 h_0}{\partial \rho_{ll} \partial \rho} \\ -\frac{\partial^2 h_0}{\partial \rho \partial \rho_{ll}} & -\left(\frac{\partial^2 h_0}{\partial \rho_{ll}^2}\right)_{\rho} \end{vmatrix} = \begin{vmatrix} -\frac{5}{2\rho} & \frac{1}{2\rho\theta} \\ \frac{1}{2\rho\theta} & -\frac{3\rho}{2\rho_{ll}^2} \end{vmatrix} = \frac{1}{6\rho^2\theta^2} > 0. \tag{2.18}$$

So the equilibrium entropy density $-h_0$ is a convex function and this is also valid in the neighborhood of the equilibrium state. In fact the second order terms are surely positive.

2.2.4 Production terms

In Extended Thermodynamics we assume that the production terms are expressed by the following linear combination of functions [Müller and Ruggeri, 2013, pag.65],

$$\begin{aligned}
\psi_{ij} &= A\delta_{ij} + B\rho_{\langle ij \rangle}, \\
\psi_{ill} &= Cq_i.
\end{aligned} \tag{2.19}$$

The arbitrary functions A , B and C are determined requiring the validity of the residual inequality (2.17) and by use of experimental data. A possible evaluation of the

functions can be obtained by comparison of (2.19) with the analogous productions computed by Jenkins and Richman [Jenkins and Richman, 1985a], where they considered a dilute granular gas that consists of smooth inelastic spheres of mass m and diameter d_p . The two authors used the Grad moment theory that was designed to study the evolution of rarefied gases and extended it to dense systems of inelastic particles. This allowed them to calculate 13-moment collisional fluxes and production terms. Below are the terms of production of stress tensor and heat flux for a rarefied granular gas

$$\begin{aligned}\psi_{ij} &= -\frac{48mv^2}{\pi d_p^2} (1 - e^2) \sqrt{\frac{\theta}{\pi}} \frac{\theta}{d_p^2} \delta_{ij} - \frac{24v(1+e)(3-e)}{5d_p} \sqrt{\frac{\theta}{\pi}} \rho \langle ij \rangle, \\ \psi_{ill} &= -\frac{4v(1+e)(49-33e)}{5d_p} \sqrt{\frac{\theta}{\pi}} q_i.\end{aligned}\quad (2.20)$$

with $v = n\pi d_p^3/6$, e the restitution coefficient and n the number density of the particles, so $\rho = nm$. Unfortunately with the productions (2.20) the residual inequality (2.17) is not always satisfied and this limits the range of validity of the field equations.

In fact we inserted the productions (2.20) into relation (2.17) to obtain the entropy production as a known function of $q = q_1$ and $\sigma = \rho_{11}$ in the one-dimensional space. Then we introduced the following dimensionless values for q and σ

$$\hat{q} = \frac{q}{\rho\theta\sqrt{\theta}} \quad \text{and} \quad \hat{\sigma} = \frac{\sigma}{d_p^2\rho^2\sqrt{\theta}\sqrt{\pi m}}, \quad (2.21)$$

so we recovered

$$\hat{\Sigma} = \frac{19-3e}{25}\hat{q}^2 + \frac{2(e+2)}{5}\hat{\sigma}^2 + 3(e-1) > 0. \quad (2.22)$$

In Fig.2.1 we showed in the $(\hat{\sigma}, \hat{q})$ -space the region in which the entropy produc-

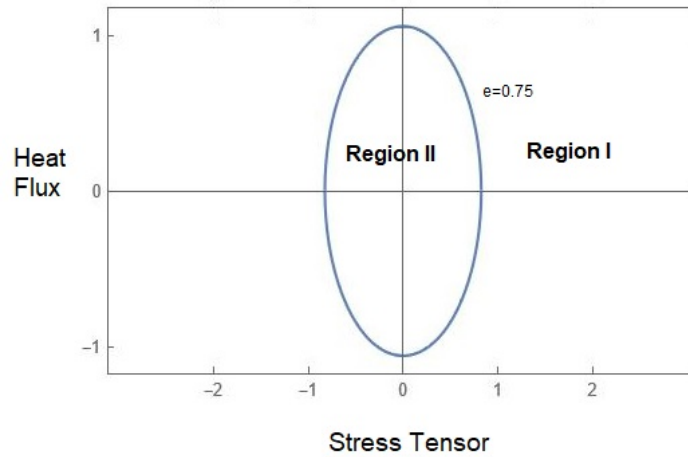


FIGURE 2.1: Study of the sign of the entropy production. In Region I the dimensionless entropy production is positive and the relation (2.22) is fulfilled, while in Region II the dimensionless entropy production is negative. These two regions are obtained with the value of the restitution coefficient $e = 0.75$

tion $\hat{\Sigma}$ is non-negative. In particular, Region I corresponds to positive entropy production, while in Region II $\hat{\Sigma}$ is negative. Thus the principle of entropy admits as acceptable values of non equilibrium variables those belonging to Region I. We also evaluated the sign of the entropy productions for different values of e as shown in Fig. 2.2. We observe that as the restitution coefficient increases towards the elastic

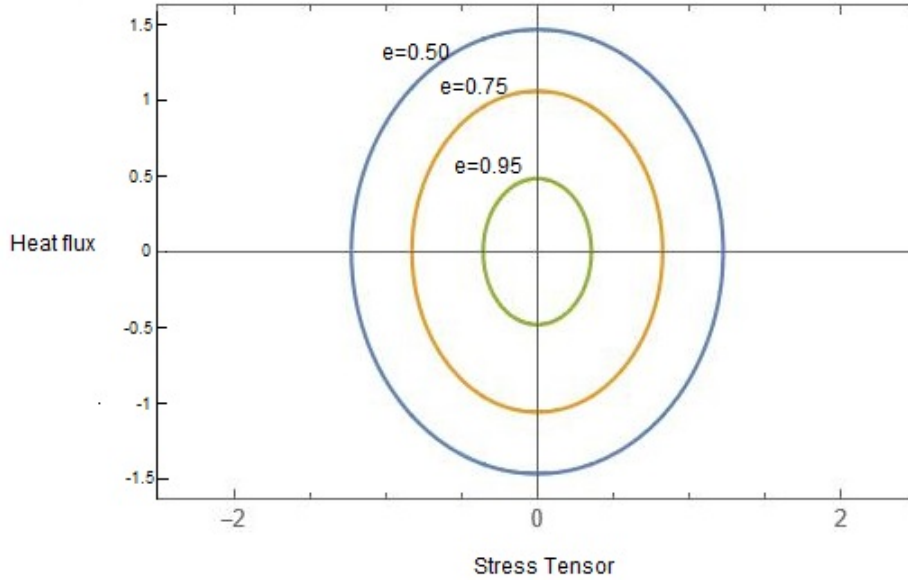


FIGURE 2.2: Study of the sign of the entropy production for different values of the restitution coefficient $e = 0.5, 0.75, 0.95$.

case, the curve becomes more and more flattened until degenerating in the elastic case. So in the elastic case the entropic production is always positive.

2.3 Hyperbolicity region

In this section we study the hyperbolicity of system (2.30), in particular we determine the boundaries of the region where system (2.30) is hyperbolic analyzing the roots of its characteristic polynomial. This limitation to hyperbolicity is due to the linear approximation made to pass from the Lagrange multipliers, such as independent variables, to physical variables. Prior to this approximation, hyperbolicity is ensured for any value of the variables [Pennisi, 2021, statement 2, pag.16 of Arima et al., 2021a].

We indicate with $\mathbf{u} = (\rho, v, \theta, \sigma, q)^T$ the field vector and suppose that each variable depends on time and the single spatial component $x = x_1$. We represent the (2.4) system in the matrix form

$$\mathbf{u}_t + A(\mathbf{u}) \mathbf{u}_x = \mathbf{f}(\mathbf{u}) \quad (2.23)$$

with the matrix of the coefficients A given by

$$A = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & \frac{1}{\rho} & 0 \\ 0 & \frac{2}{3}\left(\theta + \frac{\sigma}{\rho}\right) & v & 0 & \frac{2}{3}\frac{1}{\rho} \\ 0 & \frac{7}{3}\sigma + \frac{4}{3}\rho\theta & 0 & v & \frac{8}{15} \\ -\frac{\theta}{\rho}\sigma & \frac{16}{5}q & \frac{5}{2}(\sigma + \rho\theta) & \theta - \frac{\sigma}{\rho} & v \end{pmatrix} \quad (2.24)$$

while the vector of the production terms

$$\mathbf{f} = -\sqrt{\pi}\theta\frac{\rho}{m}d_p^2(1+e)\left(0, 0, \frac{4(1-e)}{3}\theta, \frac{4(3-e)}{5}\sigma, \frac{49-33e}{15}q\right)^T. \quad (2.25)$$

The system is hyperbolic if the matrix A is a non-singular matrix and the eigenvalue problem admits five real and distinct roots with linear independent corresponding right eigenvectors. Using the dimensionless values

$$\hat{\sigma} = \frac{\sigma}{\rho\theta}, \quad \hat{q} = \frac{q}{\rho\theta\sqrt{\theta}}, \quad \hat{\lambda} = \frac{\bar{\lambda}}{\sqrt{\theta}}, \quad (2.26)$$

with $\bar{\lambda} = \lambda - v$, the polynomial characteristic of the system (2.23) takes the form

$$\hat{\lambda} \left[\hat{\lambda}^4 - \frac{2}{15}(31\hat{\sigma} + 39)\hat{\lambda}^2 - \frac{96}{25}\hat{\lambda} + \frac{3}{5}(7\hat{\sigma}^2 + 10\hat{\sigma} + 5) \right] = 0. \quad (2.27)$$

Following [Müller and Ruggeri, 2013], we determine the boundaries of the hyperbolicity region corresponding to the case where two eigenvalues are real and coinciding, that is when the mathematical condition is verified

$$(\hat{\lambda} - \mu_1)^2(\hat{\lambda} - \mu_2)(\hat{\lambda} - \mu_3) = 0. \quad (2.28)$$

Comparing this expression with the characteristic polynomial (2.27), we recover the following relations

$$\begin{aligned} \mu_1 + \frac{1}{2}(\mu_2 + \mu_3) &= 0, \\ -\frac{2}{15}(31\hat{\sigma} + 39) + \frac{1}{2}(\mu_2 + \mu_3)^2 + \frac{1}{4}(\mu_2 - \mu_3)^2 &= 0, \\ \frac{3}{5}(7\hat{\sigma}^2 + 10\hat{\sigma} + 5) - \frac{1}{4}(\mu_2 + \mu_3)^2\mu_2\mu_3 &= 0, \\ \frac{96}{25}\hat{q} &= \pm\frac{1}{4}(\mu_2 + \mu_3)(\mu_2 - \mu_3)^2. \end{aligned} \quad (2.29)$$

These conditions are solved numerically, so it is possible to represent the heat flux \hat{q} as a function of stress tensor $\hat{\sigma}$. In Fig.2.3 we report this graph in the $(\hat{q}, \hat{\sigma})$ -space. The points of the curve correspond to the values of \hat{q} and $\hat{\sigma}$ for which there are two real and coincident eigenvalues, so the system is hyperbolic. Region I is the hyperbolicity region because the eigenvalues are all real and distinct. Region II corresponds to the case in which the eigenvalues μ_2 and μ_3 are real. In Region III the eigenvalues μ_2 and μ_3 are complex and conjugate. In conclusion, system (2.30) results no hyperbolic in Regions II and III.

As it is expected, the hyperbolic region here obtained coincide exactly with those determined for rarefied monatomic gases [Müller and Ruggeri, 2013]. In fact the left hand side of equation (2.30) coincides with the corresponding ones of a rarefied

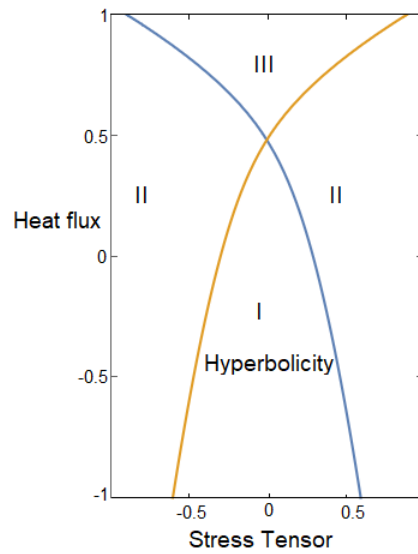


FIGURE 2.3: Hyperbolicity region in the space (σ, q)

monatomic gas. For the same reason the hyperbolic region does not depend on the restitution coefficient e . In Fig. 2.4 we represented together the hyperbolicity re-

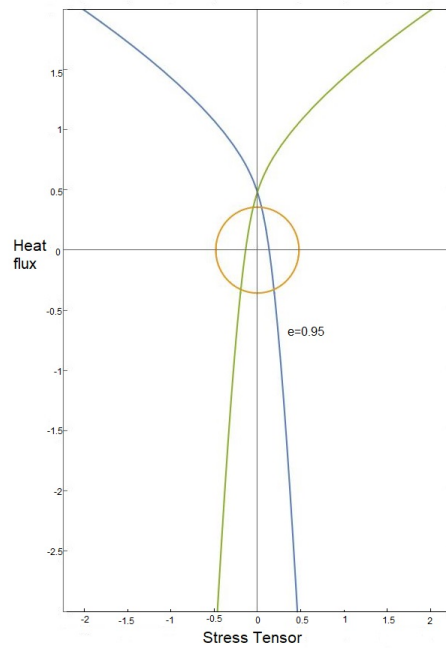


FIGURE 2.4: Hyperbolicity region and Entropy production region in the space (σ, q)

gion and the entropy production region with the value of the restitution coefficient $e = 0.95$. We observe that the common region where the system is hyperbolic and the

production of entropy is not negative is not very extensive with the choice of production terms, computed by Jenkins and Richman in [Jenkins and Richman, 1985a]. So we stress that it would be interesting to investigate the problem with other production terms to extend the region where the problem is well posed.

2.4 Field equations

Equations (2.5) together with the constitutive relations (2.11) and the productions (2.20), obtained by the Grad's model of Jenkins and Richman [Jenkins and Richman, 1985a], form a closed set of 13 fields equations for the 13 fields ρ , θ , v_i , $\rho_{\langle ij \rangle}$ and q_i . Every solution is called thermodynamic process. The closed system is therefore a partial differential equations system that is hyperbolic in the neighborhood of equilibrium. It has the following form

$$\begin{aligned}
 \frac{d\rho}{dt} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\
 \rho \frac{dv_i}{dt} + \frac{\partial(\rho\theta)}{\partial x_i} + \frac{\partial\rho_{\langle ik \rangle}}{\partial x_k} &= 0, \\
 \frac{3}{2}\rho \frac{d\theta}{dt} + \frac{\partial q_k}{\partial x_k} + \rho\theta \frac{\partial v_k}{\partial x_k} + \rho_{\langle kl \rangle} \frac{\partial v_l}{\partial x_k} &= -2 \frac{\rho^2 \sqrt{\pi\theta}}{m} d_p^2 (1 - e^2) \theta, \\
 \frac{d\rho_{\langle ij \rangle}}{dt} + \frac{4}{5} \frac{\partial q_i}{\partial x_j} - \frac{4}{15} \frac{\partial q_k}{\partial x_k} \delta_{ij} + \rho_{\langle ij \rangle} \frac{\partial v_k}{\partial x_k} + 2\rho_{\langle k(i} \frac{\partial v_{j)} }{\partial x_k} + 2\rho\theta \frac{\partial v_i}{\partial x_j} + \\
 -\frac{2}{3} \left(\rho_{\langle kl \rangle} \frac{\partial v_l}{\partial x_k} + \rho\theta \frac{\partial v_k}{\partial x_k} \right) \delta_{ij} &= -\frac{4}{5} \frac{\rho \sqrt{\pi\theta}}{m} d_p^2 (1 + e) (3 - e) \rho_{\langle ij \rangle}, \\
 \frac{dq_i}{dt} + \frac{5}{2} \frac{\partial(\rho\theta^2)}{\partial x_i} + \frac{7}{2} \frac{\partial(\theta\rho_{\langle ik \rangle})}{\partial x_k} + \frac{7}{5} q_i \frac{\partial v_k}{\partial x_k} + \frac{7}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{2}{5} q_l \frac{\partial v_l}{\partial x_i} + \\
 -\frac{\rho_{\langle il \rangle}}{\rho} \frac{\partial \rho_{\langle lk \rangle}}{\partial x_k} - \frac{\rho_{\langle ik \rangle}}{\rho} \frac{\partial(\rho\theta)}{\partial x_k} - \frac{5}{2} \theta \frac{\partial \rho_{\langle ik \rangle}}{\partial x_k} - \frac{5}{2} \theta \frac{\partial(\rho\theta)}{\partial x_i} &= \\
 = -\frac{1}{15} \frac{\rho \sqrt{\pi\theta}}{m} d_p^2 (1 + e) (49 - 33e) q_i.
 \end{aligned} \tag{2.30}$$

We aim to study its solutions in two case: the spatially homogeneous case in one dimensional space and the stationary case in one dimensional space. We verify that solutions rely in acceptable regions of hyperbolicity and non negative residual inequality and carry out some numerical applications.

2.5 Time dependent equilibrium solutions

We focus on spatially homogeneous solutions of the thirteen field equations in which the fields depend only on time. The system of field equation is

$$\begin{aligned}
 \frac{d\rho}{dt} &= 0, \\
 \frac{dv_i}{dt} &= 0, \\
 \frac{d\theta}{dt} &= -\frac{4}{3} \frac{\rho \sqrt{\pi}}{m} d_p^2 (1 - e^2) \theta^{\frac{3}{2}}, \\
 \frac{d\rho_{\langle ij \rangle}}{dt} &= -\frac{4(1+e)(3-e)}{5} \frac{\rho d_p^2 \sqrt{\pi}}{m} \theta^{\frac{1}{2}} \rho_{\langle ij \rangle}, \\
 \frac{dq_i}{dt} &= -\frac{\rho \sqrt{\pi}}{15m} d_p^2 (1 + e) (49 - 33e) \theta^{\frac{1}{2}} q_i.
 \end{aligned} \tag{2.31}$$

We observe that the mass density and the velocity field are constant in time, while the remaining equations are a set of coupled differential equations that have to be integrate to determine the temperature, the pressure tensor and the heat flux. Assuming as initial conditions, $\rho(0) = \rho_0$, $v(0) = 0$, $\theta(0) = \theta_0$, $\sigma(0) = \sigma_0$ and $q(0) = q_0$, the equations are analytically integrated providing the following expressions for density, velocity, temperature, stress tensor and heat flow:

$$\begin{aligned} \rho(t) &= \rho_0, \quad v(t) = 0, \quad \theta(t) = \frac{\theta_0}{\left(1 + \frac{2}{3} \frac{\rho_0 \sqrt{\pi} \theta_0 d_p^2 (1-e^2)}{m} t\right)^2}, \\ \sigma(t) &= \sigma_0 \left[\frac{\theta(t)}{\theta_0}\right]^{\frac{3}{5} \frac{3-e}{1-e}}, \quad q(t) = q_0 \left[\frac{\theta(t)}{\theta_0}\right]^{\frac{1}{20} \frac{49-33e}{1-e}}. \end{aligned} \quad (2.32)$$

In terms of the dimensionless-values

$$\hat{\rho} = \frac{\rho}{\rho_0}, \quad \hat{\theta} = \frac{\theta}{\theta_0}, \quad \hat{t} = \frac{t}{t_0} = \frac{t \rho_0 d_p^2 \sqrt{\theta_0}}{m}, \quad \hat{\sigma} = \frac{\sigma}{\sigma_0}, \quad \hat{q} = \frac{q}{q_0}, \quad (2.33)$$

the solution reads

$$\hat{\rho} = 1, \quad \hat{\theta} = \frac{1}{\left(1 + \frac{2\sqrt{\pi}(1-e^2)}{3} \hat{t}\right)^2}, \quad \hat{\sigma} = [\hat{\theta}(\hat{t})]^{\frac{3}{5} \frac{3-e}{1-e}}, \quad \hat{q} = [\hat{\theta}(\hat{t})]^{\frac{1}{20} \frac{49-33e}{1-e}}, \quad (2.34)$$

illustrated in Fig.2.5-2.7-2.8 for different values of the restitution coefficient e .

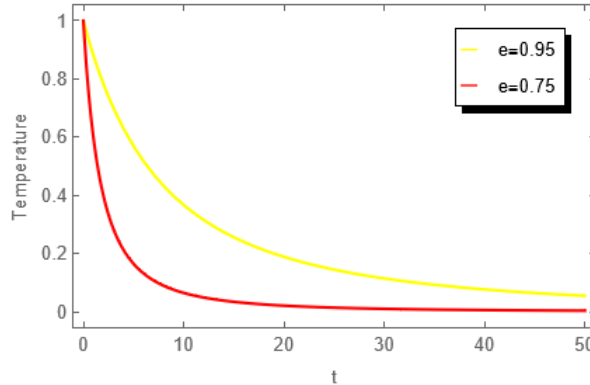


FIGURE 2.5: Temperature field obtained as solution of the homogeneous case for different values of the restitution coefficient e .

We observe in Fig.2.5 the decay of temperature for values of e that are 0.75 and 0.95. It is possible to conclude that the decay of temperature is less marked when the restitution coefficient is near to the elastic case. The behavior of the temperature is well represented by Haff's law, [Haff, 1983] that describes the dissipation of the total energy in a fluid of inelastic particles through inelastic collision:

$$\theta(t) = \frac{1}{\left\{1 + \frac{(1-e)^2}{6} \left[1 + \frac{3(1-e)(1-2e^2)}{81-17e+30e^2(1-e)}\right] t\right\}^2}. \quad (2.35)$$

The energy's decay is proportional to t^{-2} and depends on the average number of collisions suffered by a particle within time t and also on $1 - 2e^2$, that expresses the

degree of inelasticity. Kremer proved that this law defines the evolution of temperature in the fourteen model when the fourth moment remains constant in time (see for more details [Kremer and Marques Jr, 2011]). In Fig.2.6 we plotted the tempera-

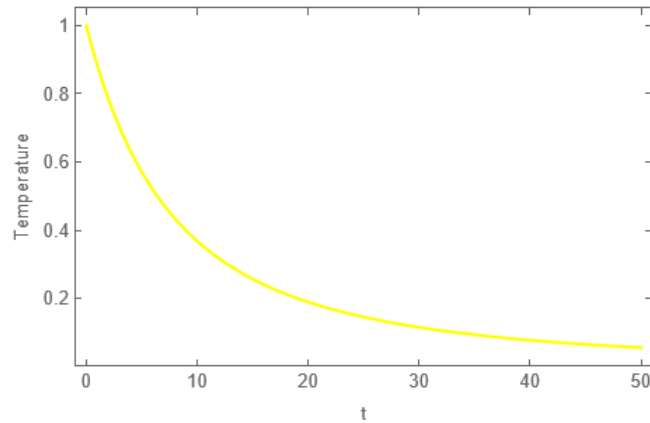


FIGURE 2.6: Temporal decay of temperature according to Haff's Law ($e=0.95$)

ture field, together with the temperature field, obtained with Haff's law for $e = 0.95$. The two graphs overlap and this confirms that Haff's law faithfully describes the temporal decay of the temperature field.

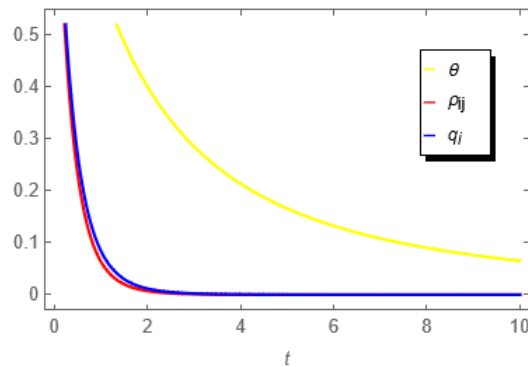


FIGURE 2.7: Temporal decays of temperature, pressure tensor and heat flux ($e=0.75$)

In Fig.2.7 we compare the decay with time of temperature, pressure tensor and heat flux when the restitution coefficient $e = 0.75$ and we notice that the pressure tensor decays faster than the other field variables and for this reason we will neglect below some terms that contain the pressure tensor. We observe in Fig.2.8 that when the restitution coefficient increases, the time decay of the pressure tensor is more marked, while the one of heat flux is more muffled. In both Figures 2.7-2.8 the temperature field decreases much more slowly than other fields.

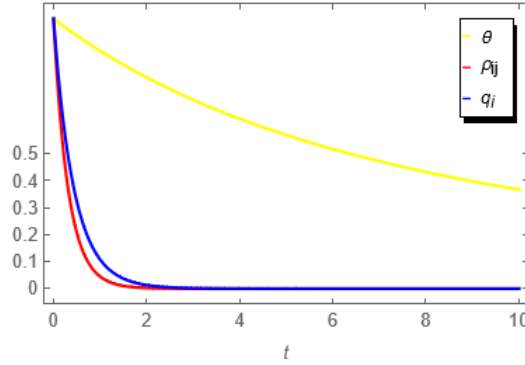


FIGURE 2.8: Temporal decays of temperature, pressure tensor and heat flux ($e=0.95$)

2.6 Dispersion relation

In this section we derive the dispersion relation relative to the system (2.30) and then we obtain the high-frequency limit of the phase velocity and the attenuation factor. Since we are interested in waves with small amplitude, we linearize the system of field equations (2.30) around the spatially homogeneous solution (2.34), determined in the previous paragraph: $\mathbf{u}_0 = (\rho_0, 0, \theta(t), \rho_{\langle ij \rangle}(t), q_i(t))$. We define the linear and dimensionless perturbations of the unknown fields:

$$\begin{aligned} \tilde{n}(x, t) &= \frac{n(x, t)}{n_0} - 1, & \tilde{v}_i(x, t) &= \frac{v_i(x, t)}{v(t)} & \tilde{\theta}(x, t) &= \frac{\theta(x, t)}{\theta(t)} - 1 \\ \tilde{\rho}_{\langle ij \rangle}(x, t) &= \frac{\rho_{ij}(x, t) - \rho_{ij}(t)}{n_0 m \theta(t)} & \tilde{q}_i(x, t) &= \frac{q_i(x, t) - q_i(t)}{n_0 m \theta(t) v(t)} \end{aligned} \quad (2.36)$$

where n_0 is the average number density of the system and $v(t) = \sqrt{\frac{5}{3}\theta(t)}$ the adiabatic sound velocity in the homogeneous cooling state. We also introduce the dimensionless quantities

$$\tilde{t} = \frac{t}{\tau(t)}, \quad \tilde{x} = \frac{x}{v(t)\tau(t)}, \quad (2.37)$$

where $\tau(t) = \frac{m}{4d_p^2 \rho \sqrt{\pi\theta(t)}}$ is the mean free time in the homogeneous cooling state.

So we substitute the relations (2.36)-(2.37) into the model (2.30). Keeping in mind the fact that the decay of the pressure tensor and heat flux are steeper than that of the temperature, we derive the following system of partial differential equations with constant coefficients:

$$\begin{aligned} \frac{\partial \tilde{n}}{\partial \tilde{t}} + \frac{\partial \tilde{v}_k}{\partial \tilde{x}_k} &= 0, \\ \frac{\partial \tilde{v}_i}{\partial \tilde{t}} + \frac{3}{5} \left(\frac{\partial \tilde{n}}{\partial \tilde{x}_i} + \frac{\partial \tilde{\theta}}{\partial \tilde{x}_i} + \frac{\partial \tilde{\rho}_{\langle ik \rangle}}{\partial \tilde{x}_k} \right) - \frac{\zeta_1}{2} \tilde{v}_i &= 0, \\ \frac{\partial \tilde{\theta}}{\partial \tilde{t}} + \frac{2}{3} \left(\frac{\partial \tilde{v}_k}{\partial \tilde{x}_k} + \frac{\partial \tilde{q}_k}{\partial \tilde{x}_k} \right) + \zeta_1 \left(\tilde{n} + \frac{\tilde{\theta}}{2} \right) &= 0, \\ \frac{\partial \tilde{\rho}_{\langle ij \rangle}}{\partial \tilde{t}} + \frac{4}{5} \frac{\partial \tilde{q}_{\langle i}}{\partial \tilde{x}_{j \rangle}} + 2 \frac{\partial \tilde{v}_{\langle i}}{\partial \tilde{x}_{j \rangle}} + \zeta_2 \tilde{\rho}_{\langle ij \rangle} &= 0, \\ \frac{\partial \tilde{q}_i}{\partial \tilde{t}} + \frac{3}{5} \frac{\partial \tilde{\rho}_{\langle ik \rangle}}{\partial \tilde{x}_k} + \frac{3}{2} \frac{\partial \tilde{\theta}}{\partial \tilde{x}_i} + \zeta_3 \tilde{q}_i &= 0 \end{aligned} \quad (2.38)$$

with

$$\zeta_1 = \frac{1-e^2}{3}, \quad \zeta_2 = 2 \frac{(1+e)(2+e)}{15}, \quad \zeta_3 = \frac{(1+e)(19-3e)}{60}. \quad (2.39)$$

In order to study the behavior of the gas for small perturbations, we assume that the fields are of the form

$$\tilde{\mathbf{U}} = \bar{\mathbf{U}} \exp [i (\omega t - \mathbf{kx})], \quad (2.40)$$

where $\mathbf{k} = (k, 0, 0)$ is the wave-vector of the perturbation and ω its angular frequency. Then we recover two independent system of linear algebraic equations for the amplitudes of the perturbations:

the longitudinal system assumes the form

$$\begin{bmatrix} \omega & -k & 0 & 0 & 0 \\ -\frac{3}{5}k & \omega + i\frac{\zeta_1}{2} & -\frac{3}{5}k & -\frac{3}{5}k & 0 \\ -i\zeta_1 & -\frac{2}{3}k & \omega - i\frac{\zeta_1}{2} & 0 & -\frac{2}{3}k \\ 0 & -\frac{4}{3}k & 0 & \omega - i\zeta_2 & -\frac{8}{15}k \\ 0 & 0 & -\frac{3}{2}k & -\frac{3}{5}k & \omega - i\zeta_3 \end{bmatrix} \begin{bmatrix} \bar{\rho} \\ \bar{v}_x \\ \bar{\theta} \\ \bar{\rho}_{\langle xx \rangle} \\ \bar{q}_x \end{bmatrix} = \mathbf{0}, \quad (2.41)$$

while the transverse system is given by

$$\begin{bmatrix} \omega + i\frac{\zeta_1}{2} & -\frac{3}{5}k & 0 \\ -k & \omega - i\zeta_2 & -\frac{2}{5}k \\ 0 & -\frac{3}{5}k & \omega - i\zeta_3 \end{bmatrix} \begin{bmatrix} \bar{v}_y \\ \bar{\rho}_{\langle xy \rangle} \\ \bar{q}_y \end{bmatrix} = \mathbf{0}. \quad (2.42)$$

It's obvious that both systems admit nontrivial solutions when the matrix determinants vanish. By imposing this condition we get the dispersion relation, through which we obtain the oscillation frequency ω as a function of the wavenumber k . Each solution of the dispersion relation detects a mode called hydrodynamic if the angular frequency ω tends to 0 when k goes to 0 and a mode called kinetic when the angular frequency tends to a constant value not zero for k going to 0. Of each solution we also study the real part of ω , which describes the oscillation frequency of the generic small perturbation with the wavenumber k and the imaginary part, which defines the temporal evolution (decay in this case or growth) of its amplitude. Solving the dispersion relation for the longitudinal system, we get 5 roots, representing precisely 4 kinetic modes and one hydrodynamic. These eigenmodes are diffusive because their real part vanishes for wavenumber values close to 0, as can be seen in Fig.2.9a). We infer that when the imaginary part of the oscillation frequency is negative, the amplitude of the perturbation decreases to 0 in time and eigenmode is said to be stable. Instead, when the imaginary part is positive, eigenmode is unstable because the amplitude of the perturbation increases temporally. The values in Fig.2.9 refer to the inelastic case, for $e=0.75$. We observe that 4 of the 5 eigenmode are stable, while the other is unstable. As for the dispersion relation of the transverse system, we observe in Fig.2.10 that in the inelastic case we have 3 modes all kinetics, whose 2 stable and one unstable.

2.7 Range of validity of the time dependent solutions

In Fig. 2.11 we plotted the time dependent solutions relating them with the hyperbolicity region and entropy production's region. In these figures we represent the

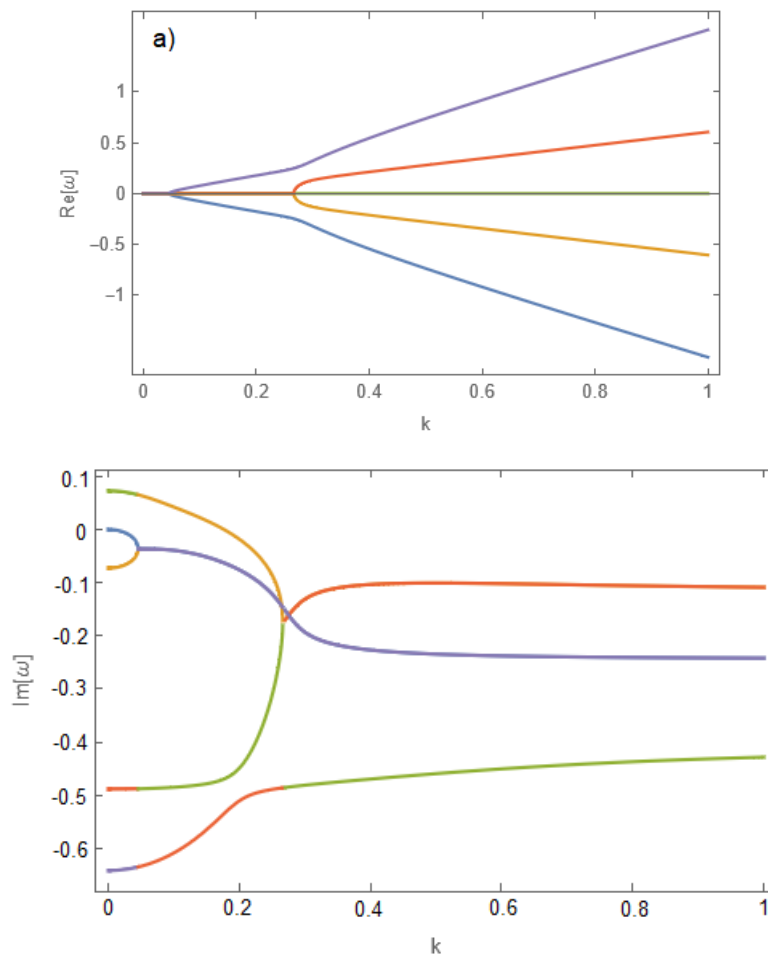
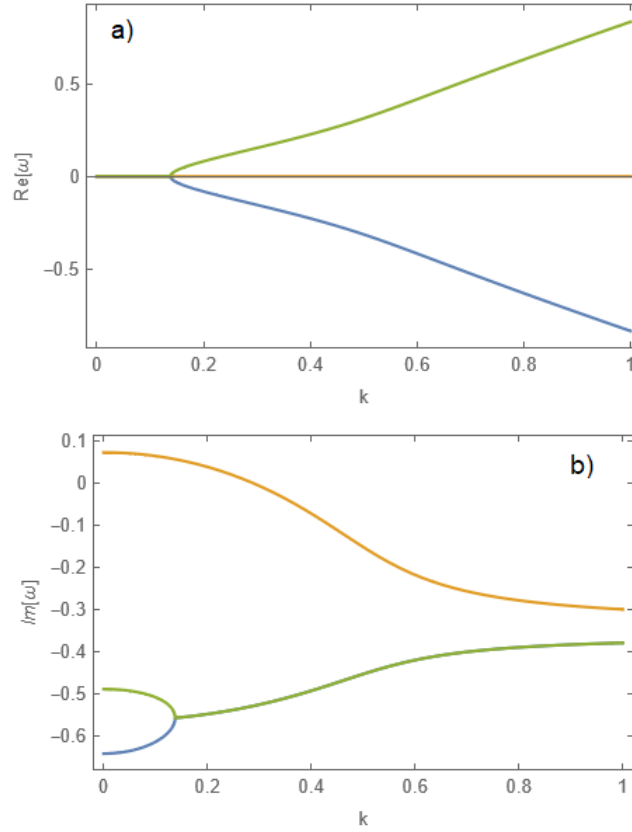


FIGURE 2.9: Real and Imaginary parts of the angular frequency for the longitudinal system ($e=0.75$)

heat flux as a curve that depends on the stress tensor. As it is possible to notice, these curves enter after some time inside the correspond ellipse, so from this time the residual inequality (2.17) is violated. For this reason the time dependent solutions can be accepted til this critical time. In addition, the region of admissibility of solutions decreases in the inelastic case, when the restitution coefficient e becomes smaller.

2.8 Stationary 1D solutions

In order to show some mathematical property of the system (2.4), we study the stationary problem of a granular gas at rest in absence of body forces. Therefore, assuming that the field variables depend only on the $x_1 = x$ -coordinate and setting


 FIGURE 2.10: Real and Imaginary parts of the angular frequency for the transverse system ($e=0.75$)

$v = 0$, it follows

$$\begin{aligned}
 \rho \frac{d\theta}{dx} + \theta \frac{d\rho}{dx} + \frac{d\sigma}{dx} &= 0, \\
 \frac{dq}{dx} &= -2 \frac{\rho d_p^2}{m} \sqrt{\pi\theta} (1 - e^2) \theta, \\
 \frac{8}{15} \frac{dq}{dx} &= -\frac{4}{5} \frac{\rho d_p^2}{m} (1 + e) (3 - e) \sqrt{\pi\theta} \sigma, \\
 \frac{5}{2} \rho \theta \frac{d\theta}{dx} + \theta \frac{d\sigma}{dx} &= -\frac{1}{15} \frac{\rho}{m} \sqrt{\pi\theta} d_p^2 (1 + e) (49 - 33e) q.
 \end{aligned} \tag{2.43}$$

Then, by manipulations of these equations one has

$$\begin{aligned}
 \rho\theta &= P, \\
 \sigma &= \frac{4}{3} \frac{1-e}{3-e} P, \\
 \frac{dq}{dx} &= -2P^2 \frac{d_p^2}{m} (1 - e^2) \sqrt{\frac{\pi}{\theta}}, \\
 \frac{d\theta}{dx} &= -\frac{2}{75} \frac{d_p^2}{m} (1 + e) (49 - 33e) \sqrt{\frac{\pi}{\theta}} q,
 \end{aligned} \tag{2.44}$$

where P is the integration constant with the dimension of a pressure.

The first two differential equations can be written as a single differential equation of 2nd order in the granular temperature, that is

$$2\theta \frac{d^2\theta}{dx^2} + \left(\frac{d\theta}{dx} \right)^2 = \frac{8}{75} \frac{\pi d_p^4 P^2}{m^2} (1 + e)^2 (1 - e) (49 - 33e). \tag{2.45}$$

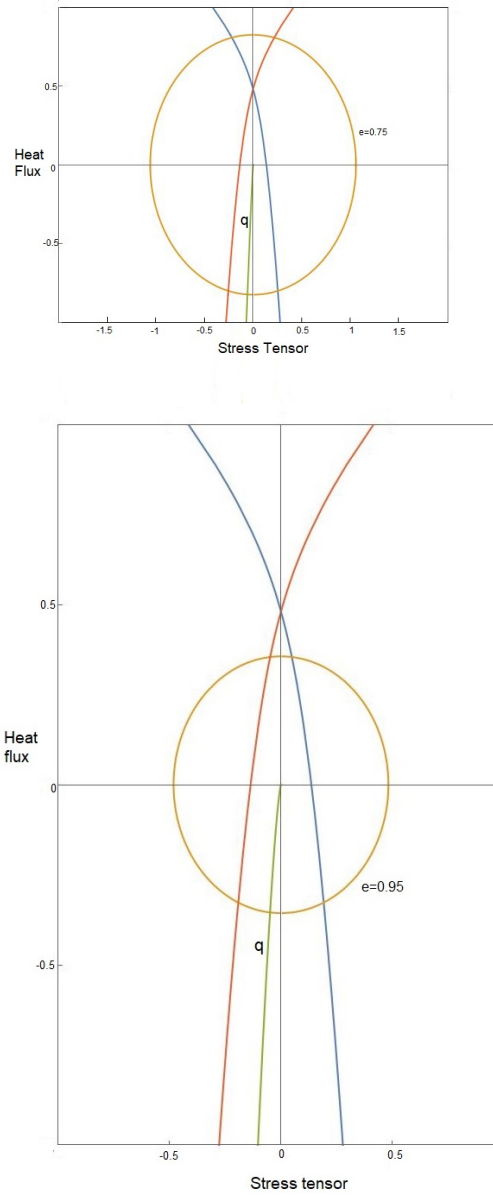


FIGURE 2.11: Range of validity of the time dependent solutions

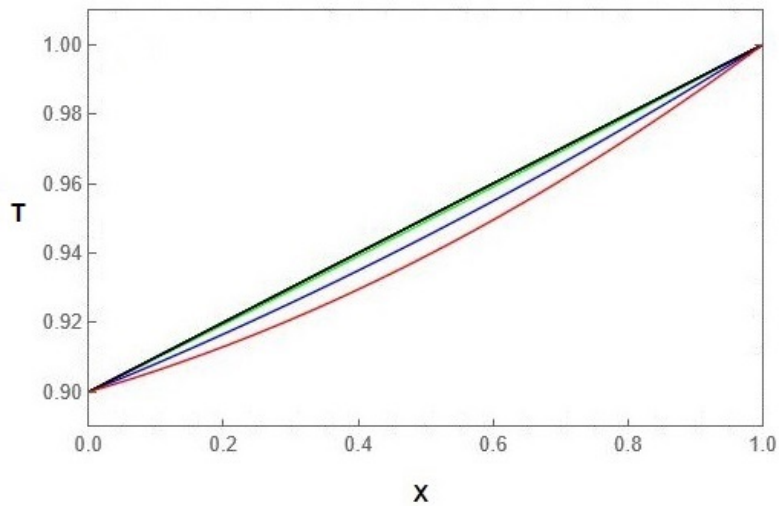
Then, for simplicity we introduce the dimensionless quantities

$$\hat{\rho} = \frac{\rho\theta_0}{P}, \quad \hat{\theta} = \frac{\theta}{\theta_0}, \quad \hat{\sigma} = \frac{\sigma}{P}, \quad \hat{q} = q \frac{m\sqrt{\theta_0}}{LP^2d_p^2}, \quad H = \frac{d_p^4 P^2 L^2}{m^2 \theta_0^2} \quad (2.46)$$

so the differential equation (2.45) becomes

$$2\hat{\theta} \frac{d^2 \hat{\theta}}{d\hat{x}^2} + \left(\frac{d\hat{\theta}}{d\hat{x}} \right)^2 = \frac{8}{75} \pi H (1+e)^2 (1-e) (49-33e). \quad (2.47)$$

The solution can be obtained in terms of known function and it is shown in Fig.2.12. Fig.2.12 shows the behavior of the granular temperature for different values of e . We observe that the granular temperature goes towards a linear behavior in the elastic case. In this kind of solution the traceless part of the stress tensor $\hat{\sigma}$ is constant, as

FIGURE 2.12: Granular temperature for different values of e .

follows from (2.44)₂. In the particular case $e = 0.95$, one has $\sigma \equiv 0.03$. Finally, it can be easily seen that, within the range of the quantities considered in this work, the solution of the differential equation (2.47) coincides with the corresponding solution of the linearized equation obtained from (2.47) neglecting the term $(d\hat{\theta}/d\hat{x})^2$.

2.9 Range of validity of the 1D solutions

In Fig. 2.13 we illustrated 1D solutions in relation with the residual inequality's region. As it can be seen the requirement of acceptability of these solutions greatly limits the range of validity of the model defined with the production terms (2.20). In fact we note that the acceptability region in which the residual inequality is not negative, that is, the area outside the ellipse, gradually narrows as the restitution coefficient decreases. For $e = 0.90$ we found that the solutions reside partially in the acceptable area.

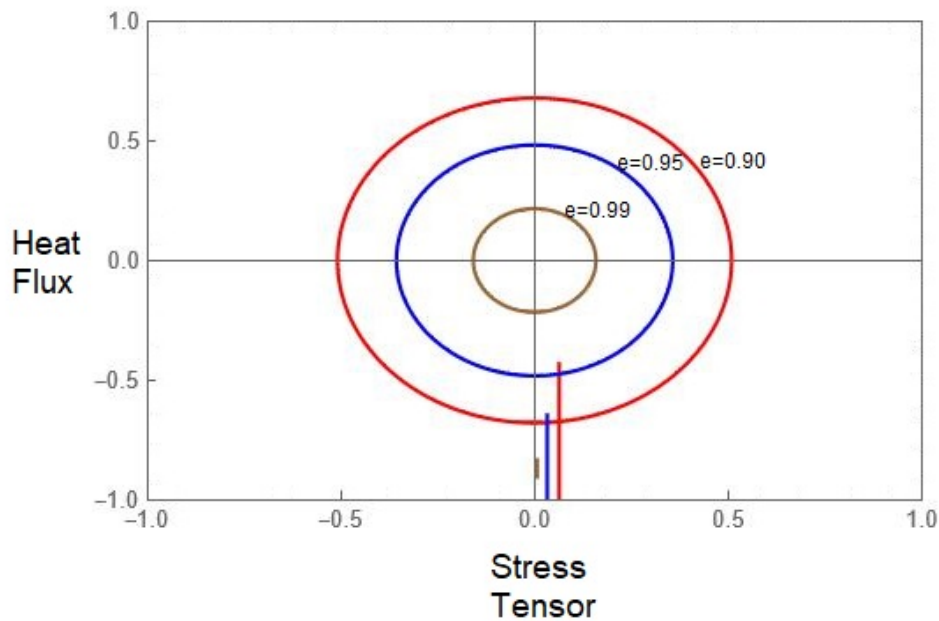


FIGURE 2.13: Range of validity of the 1D solutions

In order to avoid this limitation and to obtain more acceptable solutions of the model, more general productions than the previous productions (2.20) must be taken into account.

2.10 Conclusions and Final Remarks

This chapter is devoted to the study of granular rarefied gases, gases whose particles are very spaced and are involved in inelastic collisions. The mathematical model underlying this study is a system of 13 partial differential equations for the derivation of 13 fields, the density, the temperature, the velocity, the stress tensor and the heat flux, using the techniques of Extended Thermodynamics [Müller and Ruggeri, 2013]. The system was closed through the determination of constitutive relations of the unknown functions $\rho_{\langle ij \rangle}$, ρ_{ikll} , ψ_{ij} and ψ_{ill} . To achieve this, universal physical principles such as the Entropy Principle and the Galilean principle have been used. A first attempt was held by introducing the production terms of [Jenkins and Richman, 1985a]. The resulting system is symmetric and hyperbolic in the neighborhood of equilibrium, property that ensures from the mathematical point of view that the problem of differential equations is a well-posed Cauchy problem and from the physical point of view that the solutions have finite velocities. We determined the spatially homogeneous solutions and represented the temporal decay of temperature, relating it to Haff's law, the decay of stress tensor and heat flux in the inelastic case. Then we considered a linear perturbation of the spatially homogeneous solutions and determined the dispersion relation, studying the stability of the solutions. Moreover we determined the stationary solutions in the 1D case. The solutions for the 1D case provide non null components of the stress tensor also in the case of a gas at rest. This is in agreement with some results for stationary solutions problems in gases described by the Extended Thermodynamics (see [Barbera and Brini, 2014; Barbera and Brini, 2018]) and the references therein). The dependence of the solution

on the restitution coefficient e is shown. Unfortunately using the production terms in [Jenkins and Richman, 1985a] the range of validity of the model is very limited. A future research perspective would be to introduce suitable production terms or to study the model by adding a 14th moment and comparing solution with those obtained here. It would also be useful to compare the behavior of the temperature with the empirical law of Haff, [Haff, 1983] in relation to the 14th moment. Another application could be to treat the model using kinetic theory in order to have an exhaustive view of the behavior of granular gases and we aim to do so in future works.

Chapter 3

A Kinetic Model of 14 moments for dense gas

3.1 Introduction

The simplest case of gases that are studied in kinetic theory is represented by dilute and elastic gases, that is, gases, whose particles have positions and velocities independent of each other and they are subject to elastic collisions. In dilute gases, when two particles collide, the contribution of the other particles is not considered because they are very spaced between them. In addition, the centers of the two colliding particles are assumed to coincide. Two phenomena in binary collision can be identified: the transfer of particle properties, such as momentum and energy, and the transport of these properties. In the dilute case, the transport predominates and the transfer is neglected. In this Chapter we will focus on a more difficult case, represented by dense and granular gases: the particles have positions and velocities that depend on each other and the collisions are inelastic. This last condition implies that the kinetic energy is not conserved, but a part of it is transformed into heat and determines a dissipation of temperature. In dense gases, the positions of the centers of two colliding particles are distinguished, and in collision, the position of the two particles is affected by the presence of neighboring particles. Ultimately, the phenomenon of transfer of particle properties and transport should both be considered. Mathematically, this means that there are terms in the balance equations, related to transport and transfer, that need to be considered. Using the techniques of kinetic theory we define a fourteen moments model for dense granular gas and fluxes associated with transport, fluxes associated with transfer and and adopting approximate linear formulas [Jenkins and Richman, 1985a], we compute all the fluxes and source for each balance equation.

3.2 Definition of moments

Kinetic theory deals with non-equilibrium problems concerning gases or gas mixtures. The starting point is the distribution function that is defined in the phase space, consisting of macroscopic variables such as time and space and microscopic variables such as velocity. Precisely we infer that the function $f(t, x, c)$ is the single particle distribution function, if

$$f(t, x, c) dc \quad (3.1)$$

represents the number of particles that, at the time t , are in the position x with velocity in the range c and $c+dc$.

In terms of this function, we define the so-called moments of the distribution function

$$F_{i_1 i_2 \dots i_N}(t, \mathbf{x}) = m \int c_{i_1} c_{i_2} \dots c_{i_N} f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}, \quad (3.2)$$

with m the molecular mass. From these moments we recover the macroscopic thermodynamic quantities. In fact, the moment of zeroth and first order represent respectively the density $\rho(t, \mathbf{x})$ and the macroscopic velocity $\mathbf{v}(t, \mathbf{x})$ that are

$$\begin{aligned} \rho(t, \mathbf{x}) &= m \int f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}, \\ \rho(t, \mathbf{x}) v_i(t, \mathbf{x}) &= m \int c_i f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}. \end{aligned} \quad (3.3)$$

Then, defining the relative velocity $\mathbf{C} = \mathbf{c} - \mathbf{v}$, it is possible to introduce the internal moments as

$$\rho_{i_1 i_2 \dots i_N}(t, \mathbf{x}) = m \int C_{i_1} C_{i_2} \dots C_{i_N} f(t, \mathbf{x}, \mathbf{c}) d\mathbf{C}. \quad (3.4)$$

The first internal moments are related to well-known macroscopic quantities, that are the granular temperature, $\theta(t, \mathbf{x})$, the stress tensor ρ_{ij} and the heat flux q_i

$$\begin{aligned} \theta(t, \mathbf{x}) &= \frac{1}{3} \frac{m}{\rho} \int C^2 f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}, \\ \rho_{ij}(t, \mathbf{x}) &= m \int C_i C_j f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}, \\ q_i(t, \mathbf{x}) &= \frac{1}{2} m \int C_i C^2 f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}. \end{aligned} \quad (3.5)$$

Another quantity that will be useful later is the non equilibrium part of the so-called fourth moment, that is $\Delta(t, \mathbf{x}) = \rho_{llss} - 15\rho\theta^2$, where

$$\rho_{llss} = m \int C^4 f(t, \mathbf{x}, \mathbf{c}) d\mathbf{c}. \quad (3.6)$$

Since $c_i = C_i + v_i$, we derive the relation between the moments F and the internal moments, so we split the moments in velocity-dependent part and internal moments

$$\begin{aligned} F_{ij} &= \rho_{ij} + \rho v_i v_j, \\ F_{ijk} &= \rho_{ijk} + 3\rho_{(ij} v_k) + \rho v_i v_j v_k, \\ F_{ikll} &= \rho_{ikll} + 4\rho_{(ikl} v_l) + 6\rho_{(ik} v_l v_l) + \rho v^2 v_i v_k, \\ F_{kllss} &= \rho_{kllss} + 5\rho_{(klls} v_s) + 10\rho_{(kll} v_s v_s) + 10\rho_{(kl} v_l v_s v_s) + \rho v^4 v_k, \end{aligned} \quad (3.7)$$

and so on for moments of higher rank.

3.3 Balance equations

The distribution function $f(t, \mathbf{x}, \mathbf{c})$ obeys the Boltzmann equation

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + f_i \frac{\partial f}{\partial c_i} = \mathbf{C}(f), \quad (3.8)$$

where f_i are the specific body forces acting on the particles. The term $\mathbf{C}(f)$ is the collisional operator, that is regarded as a measure of the change of the distribution function, due to collisions between particles. The Boltzmann equation governs the evolution in time and space of the distribution function and allows us to predict

the behavior of the gas under investigation. The Boltzmann equation that examines the gas at the microscopic level returns the balance laws of Thermodynamics when we multiply it by the moments and integrate it into the space of the velocities. The purpose of this Chapter will in fact be to use the tools of kinetic theory to determine the fluxes and source terms of the balance laws and then to verify the consistency of the results obtained by comparing them with the theories of the continuous. So multiplication of the Boltzmann equation by $mc_{i_1}c_{i_2}\dots c_{i_N}$ and integration over the whole range of \mathbf{c} provide the balance equations for the macroscopic fields $F_{i_1i_2\dots i_N}(t, \mathbf{x})$, which assume the compact form

$$\frac{\partial F_{i_1i_2\dots i_N}}{\partial t} + \frac{\partial F_{ki_1i_2\dots i_N}}{\partial x_k} - NF_{(i_1i_2\dots i_{N-1})i_N} = P_{i_1i_2\dots i_N}. \quad (3.9)$$

Here the round brackets indicate the symmetric part of a tensor. The terms in the right hand side represent the productions that will be discussed later.

We assume that the gas can be described by the first fourteen moments, that are density $\rho(t, \mathbf{x})$, velocity $v_i(t, \mathbf{x})$, temperature $\theta(t, \mathbf{x})$, stress tensor $\rho_{ij}(t, \mathbf{x})$, heat flux $q_i(t, \mathbf{x})$ and the non-equilibrium part of the double trace of the moment of rank four $\Delta(t, \mathbf{x})$. Then, the balance equations for these 14 macroscopic fields are

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} &= 0, \\ \frac{\partial \rho v_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} &= \rho f_i + P_i, \\ \frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} &= 2\rho v_i f_j + P_{ij}, \\ \frac{\partial F_{ijl}}{\partial t} + \frac{\partial F_{ijkl}}{\partial x_k} &= 3F_{(il}f_l) + P_{ijl}, \\ \frac{\partial F_{llss}}{\partial t} + \frac{\partial F_{kllss}}{\partial x_k} &= 4F_{(lss}f_l) + P_{llss}. \end{aligned} \quad (3.10)$$

Equations (3.10) represent the classical hierarchy of 14 equations for classical monatomic gases [Müller and Ruggeri, 2013].

3.4 Distribution functions

The statistics of binary collisions is characterized by the complete pair distribution function $f^{(2)}(t, \mathbf{x}^1, \mathbf{c}^1, \mathbf{x}^2, \mathbf{c}^2)$, so

$$f^{(2)}(t, \mathbf{x}^1, \mathbf{c}^1, \mathbf{x}^2, \mathbf{c}^2) d\mathbf{x}^1 d\mathbf{c}^1 d\mathbf{x}^2 d\mathbf{c}^2 \quad (3.11)$$

is the probable number of pairs of particles that at the time t are located between \mathbf{x}^1 and $\mathbf{x}^1+d\mathbf{x}^1$ and \mathbf{x}^2 and $\mathbf{x}^2+d\mathbf{x}^2$ with the velocities between \mathbf{c}^1 and $\mathbf{c}^1+d\mathbf{c}^1$ and \mathbf{c}^2 and $\mathbf{c}^2+d\mathbf{c}^2$, respectively.

In the case of dilute gases, the positions and the velocities of the particles are assumed to be independent, therefore for rarefied gases one has $f^{(2)}(t, \mathbf{x}^1, \mathbf{c}^1, \mathbf{x}^2, \mathbf{c}^2) = f(t, \mathbf{x}^1, \mathbf{c}^1) f(t, \mathbf{x}^2, \mathbf{c}^2)$. For such gases the transfer of particles proprieties, like momentum and energy in collisions is neglected in comparison to the transport of particles proprieties.

For dense gases instead the transfer of particles proprieties in collisions is so important as the transport of particles proprieties. The probable position of two colliding particles is influenced by the presence of neighboring particles. To account for the interactions of neighboring particles when two particles collide, the equilibrium

value of a radial distribution function g_0 is introduced into the relation that binds $f^{(2)}$ and the velocity distribution function of each particle f ,

$$f^{(2)}(t, \mathbf{x}^1, \mathbf{c}^1, \mathbf{x}^2, \mathbf{c}^2) = g_0(x) f(t, \mathbf{x}^1, \mathbf{c}^1) f(t, \mathbf{x}^2, \mathbf{c}^2). \quad (3.12)$$

There are different evaluations of the radial distribution function g_0 , for example Charnahan and Starling [Charnahan and Starling, 1969] evaluated the probability of collision in terms of the solid volume fraction $\nu = n\pi d_p^3/6$ as

$$g_0(\nu) = \frac{1}{1-\nu} + \frac{3\nu}{2(1-\nu)^2} + \frac{\nu^2}{2(1-\nu)^3}. \quad (3.13)$$

In presence of dense gases Jenkins and Richman in [Jenkins and Richman, 1985a] showed that that the production terms can be expressed as

$$P_{i_1 i_2 \dots i_N} = \Psi_{i_1 i_2 \dots i_N} - \frac{\partial \Theta_{k i_1 i_2 \dots i_N}}{\partial x_k}. \quad (3.14)$$

The quantities $\Psi_{i_1 i_2 \dots i_N} = \Psi(m c_{i_1} c_{i_2} \dots c_{i_N})$ are defined as

$$\Psi(\psi) = \frac{1}{2} \int \int \int (\psi^{1'} + \psi^{2'} - \psi^1 - \psi^2) f^{(2)}(\mathbf{x} - d_p \mathbf{k}, \mathbf{c}^1, \mathbf{x}, \mathbf{c}^2) d_p^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \quad (3.15)$$

where ψ^i is a generic function related to the particle i . They represent the typical source terms that are already present in monatomic gases. The other terms, that are not present in kinetic theory of dilute gases, depend on the dense nature of the material under consideration. One has $\Theta_{s i_1 i_2 \dots i_N} = \Theta_s(m c_{i_1} c_{i_2} \dots c_{i_N})$ with

$$\Theta_s(\psi) = -\frac{d_p}{2} \int \int \int (\psi^{1'} - \psi^1) k_s \left(1 - \frac{d_p}{2!} k_j \frac{\partial}{\partial x_j} + \frac{d_p^2}{3!} k_j k_m \frac{\partial}{\partial x_j \partial x_m} + \dots \right) f^{(2)}(\mathbf{x}, \mathbf{c}^1, \mathbf{x} + d_p \mathbf{k}, \mathbf{c}^2) d_p^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2. \quad (3.16)$$

By substitution of (3.14) into (3.10), we get

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} &= 0, \\ \frac{\partial \rho v_i}{\partial t} + \frac{\partial}{\partial x_k} [F_{ik} + \Theta_{ik}] &= \rho f_i, \\ \frac{\partial F_{ij}}{\partial t} + \frac{\partial}{\partial x_k} [F_{ijk} + \Theta_{ijk}] &= 2\rho v_{(i} f_{j)} + \Psi_{ij}, \\ \frac{\partial F_{ill}}{\partial t} + \frac{\partial}{\partial x_k} [F_{ikll} + \Theta_{ikll}] &= 3F_{(il} f_{l)} + \Psi_{ill}, \\ \frac{\partial F_{llss}}{\partial t} + \frac{\partial}{\partial x_k} [F_{kllss} + \Theta_{kllss}] &= 4F_{(lss} f_{l)} + \Psi_{llss}. \end{aligned} \quad (3.17)$$

We take into account the internal moments (3.7) and we define the internal quantities θ and ψ as it was done for Θ and Ψ respectively, with the peculiar velocity \mathbf{C}

instead of c . Then considering the following decomposition for the production terms

$$\begin{aligned}
\Theta_{ij} &= \theta_{ij}, \\
\Theta_{ijk} &= \theta_{ijk} + 2\theta_{k(i}v_{j)}, \\
\Theta_{ikll} &= \theta_{ikll} + 3\theta_{k(il}v_l) + 3\theta_{k(i}v_l v_l), \\
\Theta_{kllss} &= \theta_{kllss} + 4\theta_{k(lls}v_s) + 6\theta_{k(ll}v_s v_s) + 4\theta_{kl}v_l v_s v_s, \\
\Psi_{ij} &= \psi_{ij}, \\
\Psi_{ill} &= \psi_{ill} + 3\psi_{(il}v_l) \\
\Psi_{ikll} &= \psi_{ikll} + 4\psi_{(ikl}v_l) + \psi_{(ik}v_l v_l),
\end{aligned} \tag{3.18}$$

one has

$$\begin{aligned}
\frac{d\rho}{dt} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\
\rho \frac{dv_i}{dt} + \frac{\partial}{\partial x_k} [\rho_{ik} + \theta_{ik}] &= \rho f_i, \\
\frac{d\rho_{ij}}{dt} + \frac{\partial}{\partial x_k} [\rho_{ijk} + \theta_{ijk}] + \rho_{ij} \frac{\partial v_k}{\partial x_k} + 2 \left[\rho_{k(i} + \theta_{k(i} \right] \frac{\partial v_j)}{\partial x_k} &= \psi_{ij}, \\
\frac{d\rho_{ill}}{dt} + \frac{\partial}{\partial x_k} [\rho_{ikll} + \theta_{ikll}] + \rho_{ill} \frac{\partial v_k}{\partial x_k} + 3 \left[\rho_{k(il} + \theta_{k(il} \right] \frac{\partial v_l}{\partial x_k} + \\
&\quad - 3 \frac{\rho_{(il}}{\rho} \frac{\partial}{\partial x_k} \left[\rho_{l)k} + \theta_{l)k} \right] &= \psi_{ill}, \\
\frac{d\rho_{llss}}{dt} + \frac{\partial}{\partial x_k} [\rho_{kllss} + \theta_{kllss}] + \rho_{llss} \frac{\partial v_k}{\partial x_k} + 4 \left[\rho_{ksll} + \theta_{ksll} \right] \frac{\partial v_s}{\partial x_k} + \\
&\quad - 8 \frac{q_l}{\rho} \frac{\partial}{\partial x_k} [\rho_{lk} + \theta_{lk}] &= \psi_{llss}.
\end{aligned} \tag{3.19}$$

The first equation represents the conservation law of mass, the second is the balance law of momentum. The quantity $\rho_{ik} + \theta_{ik}$ is the total pressure tensor: the sum of the quantity due to the transport of momentum between collisions and that transferred in collisions.

The trace of the third equation represents the balance law of energy,

$$\frac{3}{2} \rho \frac{d\theta}{dt} + \frac{1}{2} \frac{\partial}{\partial x_k} [\rho_{kll} + \theta_{kll}] + [\rho_{kl} + \theta_{kl}] \frac{\partial v_l}{\partial x_k} = \frac{1}{2} \psi_{ll}, \tag{3.20}$$

where θ is the so-called granular temperature, the sum $\frac{1}{2} [\rho_{kll} + \theta_{kll}]$ is the heat flux, with the transport and collisional parts, the last term ψ_{ll} represents the dissipation due to the inelastic nature of the collision.

The traceless part of equation (3.19)₃ assumes the form

$$\frac{d\rho_{\langle ij \rangle}}{dt} + \frac{\partial}{\partial x_k} [\rho_{\langle ij \rangle k} + \theta_{\langle ij \rangle k}] + \rho_{\langle ij \rangle} \frac{\partial v_k}{\partial x_k} + 2 [\rho_{k \langle i} + \theta_{k \langle i} \rangle] \frac{\partial v_j \rangle}{\partial x_k} = \psi_{\langle ij \rangle}. \tag{3.21}$$

Square brackets in the indexes indicate traceless part of a tensor.

3.5 Grad closure

Equations (3.19) represent a quasi linear system of 14 partial differential equations for the 14 fields ρ , v_i , θ , $\rho_{\langle ij \rangle}$, $q_k = 1/2 \rho_{kll}$ and Δ . These equations are not closed for the occurrence of the quantities $\rho_{\langle ijk \rangle}$, $\rho_{\langle ik \rangle ll}$, ρ_{kllss} , θ_{ik} , θ_{ijk} , θ_{ikll} , θ_{kllss} , ψ_{ij} , ψ_{ill} and ψ_{llss} . Following the methods of Grad [Grad, 1958], the single distribution function is

written as

$$f(t, \mathbf{x}, \mathbf{c}) = \left(1 - a_i \frac{\partial}{\partial c_i} + a_{ij} \frac{\partial^2}{\partial c_i \partial c_j} - a_{ijk} \frac{\partial^3}{\partial c_i \partial c_j \partial c_k} + \dots \right) f_0(t, \mathbf{x}, \mathbf{c}), \quad (3.22)$$

where $f_0(t, \mathbf{x}, \mathbf{c})$ is the Maxwellian distribution function given by

$$f_0(t, \mathbf{x}, \mathbf{c}) = \frac{n}{(2\pi\theta)^{\frac{3}{2}}} e^{-\frac{c^2}{2\theta}}. \quad (3.23)$$

Insertion of (3.23) into (3.22) yields the single distribution function in terms of the Hermite polynomials

$$f(t, \mathbf{x}, \mathbf{c}) = f_0 \left\{ 1 + \frac{a_i}{\theta} C_i + \frac{a_{ij}}{\theta^2} [C_i C_j - \theta \delta_{ij}] + \frac{a_{ijk}}{\theta^3} [C_i C_j C_k - 3\theta C_i \delta_{jk}] + \right. \\ \left. + \frac{a_{ijks}}{\theta^4} [C_i C_j C_k C_s - 6\theta \delta_{(ij} C_k C_s) + 3\theta^2 \delta_{ij} \delta_{ks}] + \dots \right\}. \quad (3.24)$$

The coefficients a are evaluated by insertion of (3.24), truncated to the fourth order, into the definitions of the moments (3.3, 3.5, 3.6), so it follows

$$a_i = 0, \quad a_{ij} = \frac{\rho_{<ij>}}{2\rho}, \quad a_{ijk} = \frac{q_i}{5\rho} \delta_{jk}, \quad a_{ijks} = \frac{\Delta}{120\rho} \delta_{ij} \delta_{ks}. \quad (3.25)$$

In this way, in the case of 14 moments, we obtain that the single velocity distribution function takes the form

$$f(t, \mathbf{x}, \mathbf{c}) = f_0 \left\{ 1 + \frac{\rho_{<ij>}}{2\rho\theta^2} C_i C_j + \frac{q_i C_i}{5\rho\theta^3} [C^2 - 5\theta] + \right. \\ \left. \frac{\Delta}{120\rho\theta^4} [C^4 - 10\theta C^2 + 15\theta^2] \right\}. \quad (3.26)$$

Insertion of this distribution function into the definition of the moments ρ_{ijk} , $\rho_{<ij>ll}$ and ρ_{illss} yields the constitutive relations

$$\rho_{ijk} = \frac{2}{5} (q_i \delta_{jk} + q_j \delta_{ik} + q_k \delta_{ij}), \\ \rho_{<ij>ll} = 7\theta \rho_{<ij>}, \\ \rho_{illss} = 28\theta q_i. \quad (3.27)$$

In [Jenkins and Richman, 1985a] Jenkins and Richman showed that the production terms can be evaluated from (3.15) and (3.16) obtaining

$$\psi(\varphi) = \frac{g_0(\mathbf{x})}{2} \int \int \int \Pi(\varphi) f^{(1)}(\mathbf{x}, \mathbf{c}^1) f^{(1)}(\mathbf{x}, \mathbf{c}^2) \times \\ \times \left[1 + \frac{\sigma}{2} k_i \frac{\partial}{\partial x_i} \ln \frac{f^{(1)}(\mathbf{x}, \mathbf{c}^2)}{f^{(1)}(\mathbf{x}, \mathbf{c}^1)} \right] \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2 \quad (3.28)$$

with $\Pi(\varphi) = \varphi^{1'} + \varphi^{2'} - \varphi^1 - \varphi^2$ for the source terms and

$$\theta_i(\varphi) = -\sigma \frac{g_0(\mathbf{x})}{2} \int \int \int (\varphi^{1'} - \varphi^1) k_i f^{(1)}(\mathbf{x}, \mathbf{c}^1) f^{(1)}(\mathbf{x}, \mathbf{c}^2) \times \\ \times \left[1 + \frac{\sigma}{2} k_j \frac{\partial}{\partial x_j} \left(\ln \frac{f^{(1)}(\mathbf{x}, \mathbf{c}^2)}{f^{(1)}(\mathbf{x}, \mathbf{c}^1)} \right) \right] \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2. \quad (3.29)$$

We provide approximate expression for $\theta_i(\varphi)$ and $\psi(\varphi)$ that are linear in the perturbations and the spatial gradients of velocity and temperature. So we obtain for

the 14-moment case

$$\begin{aligned}\theta_i(\varphi) &= A_i(\varphi) + B_i(\varphi) + \rho_{jk} B_{ijk}(\varphi) + q_j B_{ijll}(\varphi) + \Delta \hat{B}_i(\varphi) \\ \psi(\varphi) &= E(\varphi) + F(\varphi) + \rho_{jk} F_{jk}(\varphi) + q_j F_j(\varphi) + \Delta \hat{F}(\varphi),\end{aligned}\quad (3.30)$$

where the integrals are given by

$$\begin{aligned}A_i(\varphi) &= -\frac{\sigma}{2} g_0 \int \int \int (\varphi^{1'} - \varphi^1) k_i f_{01} f_{02} \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \\ B_i(\varphi) &= -\frac{\sigma^2}{4} g_0 \int \int \int (\varphi^{1'} - \varphi^1) k_i k_m f_{01} f_{02} \frac{\partial}{\partial x_m} \left(\ln \frac{f_{02}}{f_{01}} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \\ B_{ijk}(\varphi) &= -\frac{\sigma}{4} g_0 \int \int \int (\varphi^{1'} - \varphi^1) k_i \left(f_{01} \frac{\partial^2 f_{02}}{\partial c_i^2 \partial c_j^2} + f_{02} \frac{\partial^2 f_{01}}{\partial c_i^1 \partial c_k^1} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \\ B_{ijll}(\varphi) &= \frac{\sigma g_0}{12} \int \int \int (\varphi^{1'} - \varphi^1) k_i \left(f_{01} \frac{\partial^3 f_{02}}{\partial c_i^2 \partial c_j^2 \partial c_l^2} + f_{02} \frac{\partial^3 f_{01}}{\partial c_i^1 \partial c_j^1 \partial c_l^1} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \\ \hat{B}_i(\varphi) &= -\frac{\sigma g_0}{48} \int \int \int (\varphi^{1'} - \varphi^1) k_i \left(f_{01} \frac{\partial^4 f_{02}}{\partial c_i^2 \partial c_j^2 \partial c_s^2 \partial c_s^2} + f_{02} \frac{\partial^4 f_{01}}{\partial c_i^1 \partial c_j^1 \partial c_s^1 \partial c_s^1} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2\end{aligned}\quad (3.31)$$

and

$$\begin{aligned}E(\varphi) &= \frac{g_0}{2} \int \int \int \Pi(\varphi) f_{01} f_{02} \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \\ F(\varphi) &= \sigma \frac{g_0}{4} \int \int \int \Pi(\varphi) k_m f_{01} f_{02} \frac{\partial}{\partial x_m} \left(\ln \frac{f_{02}}{f_{01}} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \\ F_{ij}(\varphi) &= \frac{g_0}{4} \int \int \int \Pi(\varphi) \left(f_{01} \frac{\partial^2 f_{02}}{\partial c_i^2 \partial c_j^2} + f_{02} \frac{\partial^2 f_{01}}{\partial c_i^1 \partial c_j^1} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \\ F_{ijk}(\varphi) &= -\frac{g_0}{12} \int \int \int \Pi(\varphi) \left(f_{01} \frac{\partial^3 f_{02}}{\partial c_i^2 \partial c_j^2 \partial c_k^2} + f_{02} \frac{\partial^3 f_{01}}{\partial c_i^1 \partial c_j^1 \partial c_k^1} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2, \\ \hat{F}(\varphi) &= \frac{g_0}{48} \int \int \int \Pi(\varphi) \left(f_{01} \frac{\partial^4 f_{02}}{\partial c_i^2 \partial c_j^2 \partial c_s^2 \partial c_s^2} + f_{02} \frac{\partial^4 f_{01}}{\partial c_i^1 \partial c_j^1 \partial c_s^1 \partial c_s^1} \right) \sigma^2 (\mathbf{g} \cdot \mathbf{k}) d\mathbf{k} d\mathbf{c}^1 d\mathbf{c}^2\end{aligned}\quad (3.32)$$

with $f_{01} = f_0(x, c^1)$ and $f_{02} = f_0(x, c^2)$.

The integrals (3.31)₁₋₄ and (3.32)₁₋₄ are also evaluated in [Jenkins and Richman, 1985a]. We write here their values together with the new term due to the presence of the 14th moment Δ between the fields.

3.5.1 Determination of collision integrals

In order to calculate the coefficients of linear expressions (3.30), it is necessary to observe that the relations

$$Q_i^* = \frac{1}{2} \left(C_i^{(1)} + C_i^{(2)} \right) \quad \text{and} \quad g_i = C_i^{(1)} - C_i^{(2)} \quad (3.33)$$

imply the variables' change

$$C_i^{(1)} = Q_i^* + \frac{1}{2} g_i, \quad C_i^{(2)} = Q_i^* - \frac{1}{2} g_i. \quad (3.34)$$

So we have that

$$\int f_{01} f_{02} d\mathbf{c}^1 d\mathbf{c}^2 = \int \frac{n^2}{(2\pi\theta)^3} e^{-\frac{Q_i^{*2}}{\theta} - \frac{g_i^2}{4\theta}} dQ^* dg. \quad (3.35)$$

We also underline that the following term assumes the form

$$f_{01}f_{02}\frac{\partial}{\partial x_m}\left(\ln\frac{f_{02}}{f_{01}}\right) = f_{01}f_{02}\left[-\frac{g_s}{\theta}\frac{\partial v_s}{\partial x_m} - \frac{g_s Q_s^*}{\theta^2}\frac{\partial\theta}{\partial x_m}\right]. \quad (3.36)$$

so the linear decomposition of all fluxes and source terms is with respect to the unknown field: δ , $\frac{\partial v_k}{\partial x_k}$, $\frac{\partial v_{<i}}{\partial x_{>}}$, $\frac{\partial\theta}{\partial x_k}$, $\rho_{<ij>}$ and q_k . Using all the known integrals in Appendix (3.49), we obtain after cumbersome computations, all fluxes and source terms as functions of ρ , v , θ , $\rho_{<ij>}$, q_k and δ . As regards the fluxes we determine: the A_i terms, that are the equilibrium parts of fluxes,

$$\begin{aligned} A_i(mC_s) &= 2(1+e)v g_0 \rho \theta \delta_{is}, \\ A_i(mC_s C_v) &= 0, \\ A_i(mC_s C_v C_r) &= \frac{3}{5}(1+e)(10-3e+3e^2)v g_0 \rho \theta^2 \delta_{(is}\delta_{vr}), \\ A_i(mC^4) &= 0, \end{aligned} \quad (3.37)$$

the B_i terms, that are linear with respect to the derivatives $\frac{\partial v_i}{\partial x_j}$ or $\frac{\partial\theta}{\partial x_k}$,

$$\begin{aligned} B_i(mC_s) &= -\frac{2(1+e)g_0\sqrt{\pi\theta}\rho^2 d_p^4}{15m}\left(2\frac{\partial v_{(i}}{\partial x_{j)}} + \frac{\partial v_k}{\partial x_k}\delta_{ij}\right), \\ B_i(mC_s C_v) &= -\frac{2(1+e)g_0\sqrt{\pi\theta}\rho^2 d_p^4}{5m}\frac{\partial\theta}{\partial x_{(i}}\delta_{sv)}, \\ B_i(mC_s C^2) &= -\frac{(1+e)g_0\sqrt{\pi\theta}\rho^2 d_p^4}{15m}\left[(23-3e+8e^2)\frac{\partial v_{(i}}{\partial x_{j)}} + (19-4e+4e^2)\frac{\partial v_k}{\partial x_k}\delta_{ij}\right], \\ B_i(mC^4) &= -\frac{2(1+e)g_0\sqrt{\pi\theta}\rho^2 d_p^4}{3m}(13-6e+4e^2)\frac{\partial\theta}{\partial x_i}. \end{aligned} \quad (3.38)$$

the $\rho_{<jk>}B_{ijk}$ terms,

$$\begin{aligned} \rho_{<jk>}B_{ijk}(mC_s) &= \frac{2(1+e)g_0\pi\rho d_p^3}{15m}\rho_{<is>}, \\ \rho_{<jk>}B_{ijk}(mC_s C_v) &= 0, \\ \rho_{<jk>}B_{ijk}(mC_s C^2) &= \frac{(1+e)(43-21e+4e^2)g_0\pi\theta\rho d_p^3}{30m}\rho_{<is>}, \\ \rho_{<jk>}B_{ijk}(mC^4) &= 0. \end{aligned} \quad (3.39)$$

the $q_j B_{ijll}$ terms,

$$\begin{aligned} q_j B_{ijll}(mC_s) &= 0, \\ q_j B_{ijll}(mC_s C_v) &= \frac{4(1+e)g_0\pi\rho d_p^3}{75m}\left[q_i\delta_{sv} + \frac{9}{2}q_{(s}\delta_{v)i}\right], \\ q_j B_{ijll}(mC^2 C_s) &= 0, \\ q_j B_{ijll}(mC^4) &= \frac{4(1+e)(26-12e+9e^2)g_0\pi\theta\rho d_p^3}{15m}q_i, \end{aligned} \quad (3.40)$$

and the $\Delta \hat{B}_i$ terms,

$$\begin{aligned}\Delta \hat{B}_i (mC_s) &= 0, \\ \Delta \hat{B}_i (mC_s C_v) &= 0, \\ \Delta \hat{B}_i (mC^2 C_s) &= \frac{(1+e)(16-3e+3e^2)g_0\pi\rho d_p^3}{180m} \Delta \delta_{is}, \\ \Delta \hat{B}_i (mC^4) &= 0.\end{aligned}$$

Instead, as regards the source terms, we determine: the E terms, that are the equilibrium terms, that vanish for $e = 1$,

$$\begin{aligned}E (mC_s) &= 0, \\ E (mC_s C_v) &= -\frac{4(1-e^2)}{3m} g_0 \rho^2 d_p^2 \sqrt{\pi\theta} \delta_{sv}, \\ E (mC_s C_v C_r) &= 0, \\ E (mC^4) &= -\frac{4(1-e^2)(9+2e^2)}{m} g_0 \rho^2 d_p^2 \sqrt{\pi\theta} \theta^2,\end{aligned}\tag{3.41}$$

the F terms, that are linear with respect to $\frac{\partial v_i}{\partial x_j}$ or $\frac{\partial \theta}{\partial x_k}$,

$$\begin{aligned}F (mC_i) &= 0, \\ F (mC_i C_j) &= \frac{2(1+e)(2-e)}{5m} g_0 \rho^2 d_p^3 \pi \theta \frac{\partial v_{(i}}{\partial x_{j)}} + \frac{(1+e)(1-3e)}{15m} g_0 \rho^2 d_p^3 \pi \theta \frac{\partial v_k}{\partial x_k} \delta_{ij}, \\ F (mC_i C_j C_k) &= \frac{(1+e)(13-9e)}{10m} g_0 \rho^2 d_p^3 \pi \theta \delta_{(ij} \frac{\partial \theta}{\partial x_k)}, \\ F (mC^4) &= \frac{(1-e^2)(19+5e^2)}{2m} g_0 \rho^2 d_p^3 \pi \theta^2 \frac{\partial v_k}{\partial x_k},\end{aligned}\tag{3.42}$$

the $\rho_{\langle ij \rangle} F_{ij}$ terms,

$$\begin{aligned}\rho_{\langle ij \rangle} F_{ij} (mC_s) &= 0, \\ \rho_{\langle ij \rangle} F_{ij} (mC_s C_v) &= -\frac{4(1+e)(3-e)g_0\sqrt{\pi\theta}\rho d_p^2}{5m} \rho_{\langle sv \rangle}, \\ \rho_{\langle ij \rangle} F_{ij} (mC^2 C_s) &= 0, \\ \rho_{\langle ij \rangle} F_{ij} (mC^4) &= 0.\end{aligned}\tag{3.43}$$

the $q_i F_{ill}$ terms,

$$\begin{aligned}q_i F_{ill} (mC_s) &= 0, \\ q_i F_{ill} (mC_s C_v) &= 0, \\ q_i F_{ill} (mC^2 C_s) &= -\frac{2(1+e)(49-33e)g_0\sqrt{\pi\theta}\rho d_p^2}{15m} q_s, \\ q_i F_{ill} (mC^4) &= 0.\end{aligned}\tag{3.44}$$

and the $\Delta\hat{F}$ terms,

$$\begin{aligned}
\Delta\hat{F}(mC_s) &= 0, \\
\Delta\hat{F}(mC_sC_v) &= -\frac{(1-e^2)}{60m\sqrt{\theta}}g_0\rho d_p^2\sqrt{\pi\theta}\Delta\delta_{is}, \\
\Delta\hat{F}(mC^2C_s) &= 0, \\
\Delta\hat{F}(mC^4) &= -\left[\frac{(1-e^2)e^2}{2m} + \frac{(1+e)(271-207e)}{60m}\right]g_0\rho d_p^2\sqrt{\pi\theta}\Delta.
\end{aligned} \tag{3.45}$$

3.5.2 Final results

In summary, we conducted a study of dense and granular gases, determining a quasi linear model of 14 partial differential equations for 14 moments. The novelty of our work has been to determine for each balance equation the flux and the source term, based on the calculations elaborated by Jenkins and Richman [Jenkins and Richman, 1985a]. Below, then we report for each balance equation the final value of the flow term

$$\begin{aligned}
\theta_{ik} &= 2(1+e)v g_0\rho\theta\delta_{ik} - \frac{2(1+e)g_0\sqrt{\pi\theta}\rho^2d_p^4}{15m}\left(2\frac{\partial v_{(i}}{\partial x_k)} + \frac{\partial v_l}{\partial x_l}\delta_{ik}\right) + \frac{2(1+e)g_0\pi\rho d_p^3}{15m}\rho_{\langle ik\rangle}, \\
\theta_{ijk} &= -\frac{2(1+e)g_0\sqrt{\pi\theta}\rho^2d_p^4}{5m}\frac{\partial\theta}{\partial x_{(i}}\delta_{jk)} + \frac{4(1+e)g_0\pi\rho d_p^3}{75m}\left[q_i\delta_{jk} + \frac{9}{2}q_{(j}\delta_{k)i}\right], \\
\theta_{ikll} &= (1+e)(10-3e+3e^2)v g_0\rho\theta^2\delta_{ik} \\
&\quad - \frac{(1+e)g_0\sqrt{\pi\theta}\rho^2d_p^4}{15m}\left[(23-3e+8e^2)\frac{\partial v_{(i}}{\partial x_k)} + (19-4e+4e^2)\frac{\partial v_l}{\partial x_l}\delta_{ik}\right] \\
&\quad + \frac{(1+e)(43-21e+4e^2)g_0\pi\rho d_p^3}{30m}\rho_{\langle ik\rangle} + \frac{(1+e)(16-3e+3e^2)g_0\pi\rho d_p^3}{180m}\Delta\delta_{is}, \\
\theta_{kllss} &= -\frac{2(1+e)g_0\sqrt{\pi\theta}\rho^2d_p^4}{3m}(13-6e+4e^2)\frac{\partial\theta}{\partial x_k} + \frac{4(1+e)(26-12e+9e^2)g_0\pi\rho d_p^3}{15m}q_k,
\end{aligned} \tag{3.46}$$

and the final value of the source term

$$\begin{aligned}
\psi_i &= 0, \\
\psi_{ij} &= -\frac{4}{3}\frac{(1-e^2)g_0\rho^2d_p^2\sqrt{\pi\theta}}{m}\delta_{ij} + \frac{2(1+e)(2-e)g_0\rho^2d_p^3\pi\theta}{5m}\frac{\partial v_{(i}}{\partial x_j)} + \frac{(1+e)(1-3e)g_0\rho^2d_p^3\pi\theta}{15m}\frac{\partial v_k}{\partial x_k}\delta_{ij} \\
&\quad - \frac{4(1+e)(3-e)g_0\sqrt{\pi\theta}\rho d_p^2}{5m}\rho_{\langle ij\rangle} - \frac{(1-e^2)g_0\rho d_p^2\sqrt{\pi}}{60m\sqrt{\theta}}\Delta\delta_{ij}, \\
\psi_{ill} &= \frac{(1+e)(13-9e)g_0\rho^2d_p^3\pi\theta}{6m}\frac{\partial\theta}{\partial x_i} - \frac{2(1+e)(49-33e)g_0\sqrt{\pi\theta}\rho d_p^2}{15m}q_i, \\
\psi_{llss} &= -4\frac{(1-e^2)(9+2e^2)g_0\rho^2d_p^2\sqrt{\pi\theta}}{m}\theta^2 + \frac{(1-e^2)(19+5e^2)g_0\rho^2d_p^3\pi\theta^2}{2m}\frac{\partial v_k}{\partial x_k} \\
&\quad - \left[\frac{(1-e^2)e^2}{2m} + \frac{(1+e)(271-207e)}{60m}\right]g_0\rho d_p^2\sqrt{\pi\theta}\Delta.
\end{aligned} \tag{3.47}$$

Given the complexity of flux and source expressions, the next step is to refer to the stationary case (t constant and zero velocity) and to determine the spatial solutions of the model.

3.6 Appendix

To determine the previous integrals (3.46) and (3.47), it was necessary to make assumptions about the integration variables. First, indicated the orthogonal triad \mathbf{g}, \mathbf{i} and \mathbf{j} , we set the vector \mathbf{k} equal to

$$\mathbf{k} = \cos \theta \mathbf{g} + \sin \theta \cos \psi \mathbf{i} + \sin \theta \sin \psi \mathbf{j},$$

where θ is the angle between \mathbf{g} and \mathbf{k} , while ψ is the angle between \mathbf{i} and the projection of \mathbf{k} on the plane identified by \mathbf{i} and \mathbf{j} . Since it integrates in all directions of \mathbf{k} for which the relation applies $\mathbf{g} \cdot \mathbf{k} > 0$, θ varies in interval $[0, \frac{\pi}{2}]$ while ψ in the interval $[0, 2\pi]$. It is observed that if the integrand contains odd powers of $\sin \psi$ or $\cos \psi$, the integral is null. On this basis, the following integrals are obtained with respect to the variable \mathbf{k} ,

$$\begin{aligned} \int (\mathbf{g} \cdot \mathbf{k})^n d\mathbf{k} &= \frac{2\pi}{(n+1)} g^n, \\ \int (\mathbf{g} \cdot \mathbf{k})^n k_i d\mathbf{k} &= \frac{2\pi}{(n+2)} g^{n-1} g_i, \\ \int (\mathbf{g} \cdot \mathbf{k})^n k_i k_j d\mathbf{k} &= \frac{2\pi}{(n+1)(n+3)} (n g^{n-2} g_i g_j + g^n \delta_{ij}), \\ \int (\mathbf{g} \cdot \mathbf{k})^n k_i k_j k_s d\mathbf{k} &= \frac{2\pi}{(n+2)(n+4)} \left[(n-1) g^{n-3} g_i g_j g_s + 3 g^{n-1} g_{(i} \delta_{j)s} \right], \\ \int (\mathbf{g} \cdot \mathbf{k})^n k_i k_j k_s k_r d\mathbf{k} &= \frac{2\pi}{(n+1)(n+3)(n+3)} \left[n(n-2) g^{n-4} g_i g_j g_s g_r + \right. \\ &\quad \left. + 6n g^{n-2} g_{(i} g_j \delta_{sr)} + 3 g^n \delta_{(ij} \delta_{sr)} \right]. \end{aligned} \quad (3.48)$$

To make the computations easier, it was necessary to change the integration variables according to the relations

$$d\mathbf{c}_1 d\mathbf{c}_2 = d\mathbf{C}_1 d\mathbf{C}_2 = |\mathbf{J}| d\mathbf{Q}^* d\mathbf{g},$$

where $\mathbf{Q}^* = \frac{1}{2}(\mathbf{C}_1 + \mathbf{C}_2)$ and $|\mathbf{J}| = 1$. So taking into account the fundamental integral $\int e^{-x^2} dx = \pi^{\frac{3}{2}}$, the following integrals with respect to the variable \mathbf{Q}^* have to be used, some of which were calculated analytically,

$$\begin{aligned} \int e^{-\frac{Q^{*2}}{\theta}} d\mathbf{Q}^* &= \pi^{\frac{3}{2}} \theta^{\frac{3}{2}}, \\ \int Q_i^* e^{-\frac{Q^{*2}}{\theta}} d\mathbf{Q}^* &= 0, \\ \int Q_s^* Q_r^* e^{-\frac{Q^{*2}}{\theta}} d\mathbf{Q}^* &= \frac{1}{2} \pi^{\frac{3}{2}} \theta^{\frac{5}{2}} \delta_{sr}, \\ \int Q^{*2} e^{-\frac{Q^{*2}}{\theta}} d\mathbf{Q}^* &= \frac{3}{2} \pi^{\frac{3}{2}} \theta^{\frac{5}{2}}, \\ \int Q^{*2} Q_s^* Q_r^* e^{-\frac{Q^{*2}}{\theta}} d\mathbf{Q}^* &= \frac{5}{4} \pi^{\frac{3}{2}} \theta^{\frac{7}{2}} \delta_{sr}, \\ \int Q^{*4} e^{-\frac{Q^{*2}}{\theta}} d\mathbf{Q}^* &= \frac{15}{4} \pi^{\frac{3}{2}} \theta^{\frac{7}{2}}. \end{aligned} \quad (3.49)$$

As concerns the integration with respect to the variable \mathbf{g} , we have determined the following integrals,

$$\begin{aligned}
\int e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 2^3 \pi^{\frac{3}{2}} \theta^{\frac{3}{2}}, \\
\int g_s g_r e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 2^4 \pi^{\frac{3}{2}} \theta^{\frac{5}{2}} \delta_{sr}, \\
\int g_s g_r g_k g_p e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 2^5 \pi^{\frac{3}{2}} \theta^{\frac{7}{2}} (\delta_{sr} \delta_{kp} + \delta_{sk} \delta_{rp} + \delta_{sp} \delta_{rk}), \\
\int g^2 g_k g_p e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 5 \cdot 2^5 \pi^{\frac{3}{2}} \theta^{\frac{7}{2}} \delta_{kp}, \\
\int g^4 e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 3 \cdot 5 \cdot 2^5 \pi^{\frac{3}{2}} \theta^{\frac{7}{2}}, \\
\int g^2 g_s g_r g_k g_p e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 7 \cdot 2^6 \pi^{\frac{3}{2}} \theta^{\frac{9}{2}} (\delta_{sr} \delta_{kp} + \delta_{sk} \delta_{rp} + \delta_{sp} \delta_{rk}), \\
\int g^4 g_i g_j e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 5 \cdot 7 \cdot 2^6 \pi^{\frac{3}{2}} \theta^{\frac{9}{2}} \delta_{ij}, \\
\int g^6 e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 3 \cdot 5 \cdot 7 \cdot 2^6 \pi^{\frac{3}{2}} \theta^{\frac{9}{2}}, \\
\int g e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 2^5 \pi \theta^2, \\
\int g g_i g_j e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= \frac{2^8}{3} \pi \theta^3 \delta_{ij}, \\
\int g^3 e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 2^8 \pi \theta^3, \\
\int g g_i g_j g_r g_s e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= \frac{2^{10}}{5} \pi \theta^4 (\delta_{ij} \delta_{sr} + \delta_{is} \delta_{jr} + \delta_{ir} \delta_{js}), \\
\int g^3 g_r g_s e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 2^{10} \pi \theta^4 \delta_{sr}, \\
\int g^5 e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= 3 \cdot 2^{10} \pi \theta^4, \\
\int g^{-1} g_i g_j g_r g_s e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} &= \frac{2^8}{3 \cdot 5} \pi \theta^3 (\delta_{ij} \delta_{sr} + \delta_{is} \delta_{jr} + \delta_{ir} \delta_{js}).
\end{aligned} \tag{3.50}$$

$$\int g^{-1} g_i g_j g_r g_s e^{-\frac{\mathbf{g}^2}{4\theta}} d\mathbf{g} = \frac{2^8}{3 \cdot 5} \pi \theta^3 (\delta_{ij} \delta_{sr} + \delta_{is} \delta_{jr} + \delta_{ir} \delta_{js}). \tag{3.51}$$

We observe that in the previous relations integrals with an odd number of functions g do not appear, because they integrate to zero.

3.7 Concluding remarks

In this Chapter we started from the Grad's 13 model for dense and granular gases of Jenkins and Richman [Jenkins and Richman, 1985a] and we extended it to a model of 14 moments, adding the 14th scalar moment Δ and the balance equation corresponding to it. The θ_i fluxes, related to the transfer of the particle moments and the ψ source terms for each balance equation have been analytically determined, generalizing linear approximations with respect to the unknown fields, elaborated by Jenkins and Richman in [Jenkins and Richman, 1985a]. A future research perspective would be to treat the model on the basis of continuum thermodynamic theories, in particular the Rational Extended Thermodynamics, that is a macroscopic discipline that is based on the results of the kinetic theory and on the method of Grad thirteen moments. It would be interesting to make numerical applications such as the propagation of discontinuity waves from stationary or spatially homogeneous solutions and the study of the hyperbolicity region of the model in the neighborhood of the equilibrium, as we made in the paper [Barbera E, 2023] for rarefied granular

gases. Finally, we observe that the model of the 14 moments that we have defined is a system of differential equations that can be expressed in the matrix form

$$C(u)u_{xx} + u_t + A(u)u_x = D(u), \quad (3.52)$$

with $C(u), A(u), D(u)$ matrices. It is therefore clear that it is a parabolic system, which has the disadvantage of not having a limit for the speed of propagation of its solutions. A future perspective could be to modify the 14-moment model to make it hyperbolic, in order to study it in the context of Rational Extended Thermodynamics.

Chapter 4

An Extended Thermodynamic Model of 13 moments for moderately dense granular gas

4.1 Introduction

Moderately dense granular gases are gases in which particles are subject to inelastic collisions and in binary collision the centers of the two particles are distinct and interactions with neighboring particles must be taken into account. In the previous chapter we defined a quasi linear model of 14 differential equations for 14 moments, where fluxes and source terms were determined with the techniques of kinetic theory. It is precisely the term of flux $\theta_{ki_1, \dots, i_N}$ that indicates the dense character of gases. In this chapter we derive a quasi linear model of 13 differential equations for 13 moments in the context of extended thermodynamics using the fluxes and production terms computed in the previous chapter.

4.2 Balance equations

For the description of a moderately dense granular gas, we consider a model of 13 differential equations

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} &= 0, \\ \frac{\partial \rho v_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} &= \rho f_i + P_i, \\ \frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} &= 2\rho v_i f_j + P_{ij}, \\ \frac{\partial F_{ill}}{\partial t} + \frac{\partial F_{ikll}}{\partial x_k} &= 3F_{(il} f_l) + P_{ill}, \end{aligned} \tag{4.1}$$

where the unknown fields are the density $\rho(t, \mathbf{x})$, the velocity $v_i(t, \mathbf{x})$, the temperature $\theta(t, \mathbf{x})$, the stress tensor $\rho_{ij}(t, \mathbf{x})$ and the heat flux $q_i(t, \mathbf{x})$. and P are the production terms. The set (4.1) represents the classical hierarchy of 13 equations for monoatomic gases [Müller and Ruggeri, 2013]. In presence of dense gases of inelastic spheres, it has been shown by Jenkins and Richman [Jenkins and Richman, 1985a] that production terms take into account two subsidies,

$$P_{i_1 i_2 \dots i_N} = \Psi_{i_1 i_2 \dots i_N} - \frac{\partial \Theta_{ki_1 i_2 \dots i_N}}{\partial x_k}. \tag{4.2}$$

The quantities $\psi_{i_1 i_2 \dots i_N}$ represent the typical source terms that are already present in monoatomic gases, while the terms $\theta_{ki_1, \dots, i_N}$ take into account the dense nature of the material under consideration.

By substitution of (4.2) into (4.1), we get

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} &= 0, \\
 \frac{\partial \rho v_i}{\partial t} + \frac{\partial}{\partial x_k} [F_{ik} + \Theta_{ik}] &= \rho f_i, \\
 \frac{\partial F_{ij}}{\partial t} + \frac{\partial}{\partial x_k} [F_{ijk} + \Theta_{ijk}] &= 2\rho v_{(i} f_{j)} + \Psi_{ij}, \\
 \frac{\partial F_{ill}}{\partial t} + \frac{\partial}{\partial x_k} [F_{ikll} + \Theta_{ikll}] &= 3F_{(il} f_{l)} + \Psi_{ill}.
 \end{aligned} \tag{4.3}$$

The system of field equations (4.3) is not closed, since there are constitutive quantities that have to be expressed as known functions of the fields variables. In this Chapter we adopt the methods of Rational Extended Thermodynamics in order to derive the constitutive functions and to determine the solutions of the model.

4.3 Galilean invariance

We require that the balance equations (4.3) hold in every inertial frame, so that they must be invariant under a Galilean transformation. This requirement enables us to split the moments, the fluxes and the production terms of (4.3) into convective and non convective parts. So we obtain for moments and fluxes

$$\begin{aligned}
 F_{ij} &= \rho_{ij} + \rho v_i v_j, \\
 F_{ijk} &= \rho_{ijk} + 3\rho_{(ij} v_{k)} + \rho v_i v_j v_k, \\
 F_{ikll} &= \rho_{ikll} + 4\rho_{(ikl} v_{l)} + 6\rho_{(ik} v_l v_{l)} + \rho v^2 v_i v_k,
 \end{aligned} \tag{4.4}$$

while for production terms

$$\begin{aligned}
 \Theta_{ij} &= \theta_{ij}, \\
 \Theta_{ijk} &= \theta_{ijk} + 2\theta_{k(i} v_{j)}, \\
 \Theta_{ikll} &= \theta_{ikll} + 3\theta_{k(il} v_{l)} + 3\theta_{k(i} v_l v_{l)}, \\
 \Psi_{ij} &= \psi_{ij}, \\
 \Psi_{ill} &= \psi_{ill} + 3\psi_{(il} v_{l)}.
 \end{aligned} \tag{4.5}$$

By substitution of (4.4) and (4.5) into the balance equations (4.3) we recover a more compact form of the equations, that is

$$\begin{aligned}
 \frac{d\rho}{dt} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\
 \rho \frac{dv_i}{dt} + \frac{\partial}{\partial x_k} [\rho_{ik} + \theta_{ik}] &= \rho f_i, \\
 \frac{d\rho_{ij}}{dt} + \frac{\partial}{\partial x_k} [\rho_{ijk} + \theta_{ijk}] + \rho_{ij} \frac{\partial v_k}{\partial x_k} + 2 \left[\rho_{k(i} + \theta_{k(i} \right] \frac{\partial v_{j)}}{\partial x_k} &= \psi_{ij}, \\
 \frac{d\rho_{ill}}{dt} + \frac{\partial}{\partial x_k} [\rho_{ikll} + \theta_{ikll}] + \rho_{ill} \frac{\partial v_k}{\partial x_k} + 3 \left[\rho_{k(il} + \theta_{k(il} \right] \frac{\partial v_l}{\partial x_k} + \\
 -3 \frac{\rho_{(il}}{\rho} \frac{\partial}{\partial x_k} [\rho_{l)k} + \theta_{l)k}] &= \psi_{ill}.
 \end{aligned} \tag{4.6}$$

Of course the first equation represents the conservation law of mass while the second is the balance law of momentum. The quantity $P_{ik} = \rho_{ik} + \theta_{ik}$ is the total

pressure tensor: the sum of the quantity due to the transport of momentum between collisions and that transferred in collisions.

The trace of the equation (4.6)₃ is the balance law of energy

$$\frac{3}{2}\rho \frac{d\theta}{dt} + \frac{1}{2} \frac{\partial}{\partial x_k} [\rho_{kll} + \theta_{kll}] + [\rho_{kl} + \theta_{kl}] \frac{\partial v_l}{\partial x_k} = \frac{1}{2} \psi_{ll}, \quad (4.7)$$

where θ is the so-called granular temperature, the sum $Q_k = \frac{1}{2} [\rho_{kll} + \theta_{kll}]$ is the heat flux, with the transport and collisional parts and the last term ψ_{ll} represents the dissipation due to the inelastic nature of the collision.

The traceless part of equation (4.6)₃ assumes the form

$$\frac{d\rho_{\langle ij \rangle}}{dt} + \frac{\partial}{\partial x_k} [\rho_{\langle ij \rangle k} + \theta_{\langle ij \rangle k}] + \rho_{\langle ij \rangle} \frac{\partial v_k}{\partial x_k} + 2 [\rho_{k \langle i} + \theta_{k \langle i}] \frac{\partial v_{j \rangle}}{\partial x_k} = \psi_{\langle ij \rangle}. \quad (4.8)$$

Square brackets in the indexes indicate traceless part of a tensor.

The model (4.6) consists of 13 equations for the 13 fields ρ , v_i , θ , $\rho_{\langle ij \rangle}$ and $q_k = 1/2 \rho_{kll}$. Unfortunately, these equations are not closed for the occurrence of the constitutive quantities $\rho_{\langle ijk \rangle}$, ρ_{ikll} , θ_{ik} , θ_{ijk} , θ_{ikll} , ψ_{ij} and ψ_{ill} .

4.4 Entropy principle

The entropy principle asserts the existence of the concave entropy density h , the entropy flux h_k and the entropy production Σ such that the balance law

$$\frac{\partial h}{\partial t} + \frac{\partial h_k}{\partial x_k} = \Sigma \geq 0 \quad (4.9)$$

must be valid for all thermodynamic process, that is for all solutions of the field equations (4.6). In this way, equations (4.6) can be considered as constrains for the validity of the entropy principle. Following the methods of Extended Thermodynamics, we take into account theses constrains by introducing the so-called Lagrange Multipliers [Liu, 1972], so we have

$$\begin{aligned} & \frac{\partial h}{\partial t} + \frac{\partial h_k}{\partial x_k} + \\ & -\lambda \left[\frac{d\rho}{dt} + \rho \frac{\partial v_k}{\partial x_k} \right] + \\ & -\lambda_i \left[\rho \frac{dv_i}{dt} + \frac{\partial}{\partial x_k} [\rho_{ik} + \theta_{ik}] - \rho f_i \right] + \\ & -\lambda_{ij} \left[\frac{d\rho_{ij}}{dt} + \frac{\partial}{\partial x_k} [\rho_{ijk} + \theta_{ijk}] + \rho_{ij} \frac{\partial v_k}{\partial x_k} + 2 [\rho_{k(i} + \theta_{k(i)}] \frac{\partial v_{j)}}{\partial x_k} - \psi_{ij} \right] + \\ & -\lambda_{ill} \left[\frac{d\rho_{ill}}{dt} + \frac{\partial}{\partial x_k} [\rho_{ikll} + \theta_{ikll}] + \rho_{ill} \frac{\partial v_k}{\partial x_k} + 3 [\rho_{k(il} + \theta_{k(il)}] \frac{\partial v_l}{\partial x_k} + \right. \\ & \quad \left. - 3 \frac{\rho_{(il}}{\rho} \frac{\partial}{\partial x_k} [\rho_{l)k} + \theta_{l)k}] - \psi_{ill} \right] = \Sigma \geq 0 \end{aligned} \quad (4.10)$$

that must be valid for all fields. The entropy quantities and the Lagrange multipliers must be expressed as functions of the fields, in particular the entropy flux with the requirement of Galilean invariance becomes

$$h_k = hv_k + \phi_k. \quad (4.11)$$

Furthermore, since we are interested in processes not far away the equilibrium state characterized by vanishing fluxes $\rho_{\langle ik \rangle}$ and q_i , we develop the entropy density, the entropy flux and the Lagrange multipliers in the neighborhood of the equilibrium state, that is

$$\begin{aligned}
 h &= h_0(\rho, \theta) + h_1 \rho_{\langle ij \rangle} \rho_{\langle ij \rangle} + h_2 q_i q_i, \\
 \phi_k &= \phi_1 q_k + \phi_2 \rho_{\langle lk \rangle} q_l, \\
 \lambda &= \lambda_0 + \lambda_1 \rho_{\langle ij \rangle} \rho_{\langle ij \rangle} + \lambda_2 q_l q_l, \\
 \lambda_i &= \omega_1 q_i + \omega_2 \rho_{\langle il \rangle} q_l, \\
 \lambda_{ij} &= \nu_0 \delta_{ij} + \nu_1 \rho_{\langle ij \rangle} + \nu_2 \rho_{\langle il \rangle} \rho_{\langle lj \rangle} + \nu_3 q_i q_j, \\
 \lambda_{ill} &= \sigma_1 q_i + \sigma_2 \rho_{\langle il \rangle} q_l
 \end{aligned} \tag{4.12}$$

and the constitutive variables

$$\begin{aligned}
 \rho_{ijk} &= \frac{2}{5} q_i \delta_{jk} + O(2), \\
 \rho_{ijll} &= \gamma_0 \delta_{ij} + \gamma_1 \rho_{\langle ij \rangle} + O(2).
 \end{aligned} \tag{4.13}$$

At equilibrium we have

$$dh_0 = \lambda_0 d\rho + \nu_0 d\rho_{ll} = \lambda_0 d\rho + 2\nu_0 d[\rho e] \tag{4.14}$$

with e the specific internal energy. By comparison with the Gibbs equation we get

$$\nu_0 = \frac{1}{2\theta} \quad \text{and} \quad \lambda_0 = -\frac{g}{\theta}, \tag{4.15}$$

where $g = e - \theta \frac{h_0}{\rho} + \frac{p}{\rho}$ is the specific free enthalpy or Gibbs free energy.

The remaining fields become

$$\begin{aligned}
 h &= h_0(\rho, \theta) - \frac{1}{4\rho\theta^2} \rho_{\langle ij \rangle} \rho_{\langle ij \rangle} - \frac{1}{5\rho^2\theta^3} q_i q_i, \\
 \phi_k &= \frac{1}{\theta} q_k - \frac{2}{5\rho\theta^2} \rho_{\langle lk \rangle} q_l, \\
 \lambda &= -\frac{g}{\theta} - \frac{1}{4\rho^2\theta^2} \rho_{\langle ij \rangle} \rho_{\langle ij \rangle} - \frac{2}{5\rho^2\theta^5} q_l q_l, \\
 \lambda_i &= 0, \\
 \lambda_{ij} &= \frac{1}{2\theta} \delta_{ij} - \frac{1}{2\rho\theta^2} \rho_{\langle ij \rangle} + \frac{1}{2\rho^2\theta^3} \rho_{\langle il \rangle} \rho_{\langle lj \rangle} + \frac{3}{5\rho^2\theta^4} q_i q_j, \\
 \lambda_{ill} &= -\frac{1}{5\rho\theta^3} q_i + \frac{9}{25\rho^2\theta^4} \rho_{\langle il \rangle} q_l
 \end{aligned} \tag{4.16}$$

with the constitutive functions

$$\begin{aligned}
 \rho_{ijk} &= \frac{2}{5} q_i \delta_{jk} + O(2), \\
 \rho_{ijll} &= 5\rho\theta^2 \delta_{ij} + 7\theta \rho_{\langle ij \rangle} + O(2).
 \end{aligned} \tag{4.17}$$

We obtain the residual inequality of entropy,

$$\begin{aligned}
 &-\lambda_{ij} \left[\frac{\partial \theta_{ijk}}{\partial x_k} + 2\theta_{k(i} \frac{\partial v_j)}{\partial x_k} \right] - \lambda_{ill} \left[\frac{\partial \theta_{ikll}}{\partial x_k} + 3\theta_{k(il} \frac{\partial v_l)}{\partial x_k} - 3 \frac{\rho_{(il}}{\rho} \frac{\partial \theta_{l)k}}{\partial x_k} \right] = \\
 &= \Sigma - \lambda_{ij} \psi_{ij} - \lambda_{ill} \psi_{ill} \geq 0.
 \end{aligned} \tag{4.18}$$

4.5 Production terms

In this section we represent the productions terms as linear expressions with respect to the non-equilibrium variables $\rho_{\langle ij \rangle}$ and q_i , so we have

$$\begin{aligned}\theta_{ij} &= \alpha_0 \delta_{ij} + \alpha_1 \rho_{\langle ij \rangle}, \\ \theta_{ijk} &= 3\beta_1 q_i \delta_{jk}, \\ \theta_{ijll} &= \gamma_0 \delta_{ij} + \gamma_1 \rho_{\langle ij \rangle}\end{aligned}\quad (4.19)$$

and

$$\begin{aligned}\psi_{ij} &= A_0 \delta_{ij} + A_1 \rho_{\langle ij \rangle}, \\ \psi_{ill} &= B_1 q_i.\end{aligned}\quad (4.20)$$

These expressions are recovered through the macroscopic model, but more restrictive expressions can be obtained using the kinetic model [see eq. (50) of Arima et al., 2021b]. As already said in Chapter 2 the coefficients A_0 , A_1 and B_1 must be determined using experimental values and according to the residual inequality that in this case is given by (4.18). For simplicity we recover here the coefficients A_0 , A_1 and B_1 using the calculations of [Jenkins and Richman, 1985a]. This can limit also here the range of validity of solutions. Clearly our model can support other different values of these unknown coefficients. We recover the coefficient terms by comparison with the coefficients obtained by Jenkins et al. in [Jenkins and Richman, 1985a].

First of all, using the productions (4.19) and (4.20), we obtain the conservation law of mass, the balance laws for momentum and energy,

$$\begin{aligned}\frac{d\rho}{dt} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\ \rho \frac{dv_i}{dt} + \frac{\partial}{\partial x_i} [p + \alpha_0] + \frac{\partial}{\partial x_k} [(1 + \alpha_1) \rho_{\langle ij \rangle}] &= \rho f_i, \\ 3\rho \frac{d\theta}{dt} + 2 \frac{\partial}{\partial x_k} [(1 + \frac{5}{2}\beta_1) q_k] + 2(p + \alpha_0) \frac{\partial v_k}{\partial x_k} + \\ &+ 2(1 + \alpha_1) \rho_{\langle lk \rangle} \frac{\partial v_l}{\partial x_k} = 3A_0,\end{aligned}\quad (4.21)$$

the balance equation for the stress tensor,

$$\begin{aligned}\frac{d\rho_{\langle ij \rangle}}{dt} + \frac{4}{5} \frac{\partial}{\partial x_{\langle i}} [(1 + \frac{5}{2}\beta_1) q_{j \rangle}] + \rho_{\langle ij \rangle} \frac{\partial v_k}{\partial x_k} + \\ + 2(p + \alpha_0) \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} + 2(1 + \alpha_1) \rho_{k \langle i} \frac{\partial v_{j \rangle}}{\partial x_k} = A_1 \rho_{\langle ij \rangle}\end{aligned}\quad (4.22)$$

and the balance equation for the heat flux,

$$\begin{aligned}2 \frac{dq_i}{dt} + \frac{\partial}{\partial x_i} [5\rho\theta^2 + \gamma_0] + \frac{\partial}{\partial x_k} [(7\theta + \gamma_1) \rho_{\langle ik \rangle}] + \\ + 2(\frac{2}{5} + \beta_1) \left[q_i \frac{\partial v_k}{\partial x_k} + q_l \frac{\partial v_l}{\partial x_i} + \frac{7}{2} q_k \frac{\partial v_i}{\partial x_k} \right] + 2q_i \frac{\partial v_k}{\partial x_k} + \\ - \left[2 \frac{\rho_{\langle il \rangle}}{\rho} + 5 \frac{\rho\theta\delta_{il}}{\rho} \right] \left[\frac{\partial}{\partial x_l} (p + \alpha_0) + \frac{\partial}{\partial x_k} ((1 + \alpha_1) \rho_{\langle lk \rangle}) \right] = B_1 q_i\end{aligned}\quad (4.23)$$

The first coefficient A_0 is related to the dissipation of energy, indeed considering spatially homogeneous fields we have the following equations for the decay of temperature

$$\rho \frac{d\theta}{dt} = A_0, \quad (4.24)$$

that was also obtained and studied in [Kremer and Marques Jr, 2011] and [Barbera E, 2023]. Then by comparison with [Jenkins and Richman, 1985a], it is possible to identify A_0 as

$$A_0 = -\frac{4(1-e^2)g_0\rho^2d_p^2\sqrt{\pi\theta}}{3m}. \quad (4.25)$$

By substitution of (4.25) into the differential equations (4.24), we obtain the time dependence of the granular temperature that takes into consideration the energy dissipation due to the inelastic collision by means of the restitution coefficient e . This time evolution law is expressed by the Haff law [Haff, 1983] and described by many authors [Brilliantov and Pöschel, 2004; Kremer and Marques Jr, 2011; Gupta, Shukla, and Torrilhon, 2018b].

Then we determine the relaxation times, that, following [Jenkins and Richman, 1985a], can be identified as the two coefficients τ_ρ and τ_q such that the deviatoric part of the stress tensor and the heat flux decay to zero exponentially with these two coefficients. This means that in the homogeneous case must be valid

$$\begin{aligned} \frac{d\rho_{\langle ij \rangle}}{dt} &= -\frac{\rho_{\langle ij \rangle}}{\tau_\rho}, \\ \frac{dq_i}{dt} &= -\frac{q_i}{\tau_q}. \end{aligned} \quad (4.26)$$

By comparison of (4.26) with the homogeneous equations obtained by (4.22,4.23) and the corresponding values evaluated by the kinetic theory one has

$$\begin{aligned} A_1 &= -\frac{1}{\tau_\rho} = -\frac{4(1+e)(3-e)g_0\sqrt{\pi\theta}\rho d_p^2}{5m}, \\ B_1 &= -\frac{1}{2\tau_q} = -\frac{(1+e)(49-33e)g_0\sqrt{\pi\theta}\rho d_p^2}{15m}. \end{aligned} \quad (4.27)$$

We proceed now with the first Maxwellian iteration, that can be obtained inserting the equilibrium term in the left hand side of the equations, so we have

$$\begin{aligned} 2\rho\theta\frac{\partial v_{\langle i}}{\partial x_{j \rangle}} &= -|A_1|\rho_{\langle ij \rangle}, \\ 5\rho\theta\frac{\partial \theta}{\partial x_i} &= -|B_1|q_i. \end{aligned} \quad (4.28)$$

So we obtain the classical Navier-Stokes Fourier laws for the stress tensor and the heat flux, with explicit expressions for the viscosity and the heat conductivity, that are

$$\mu = \frac{\rho\theta}{|A_1|} \quad \text{and} \quad k = \frac{5\rho\theta}{|B_1|}. \quad (4.29)$$

Comparing (4.19) and (4.20) with corresponding productions obtained in the Grad's 13 moments theory, we can identify

$$\begin{aligned} \alpha_0 &= 2(1+e)vg_0\rho\theta, \\ \gamma_0 &= (1+e)(10-3e+3e^2)vg_0\rho\theta^2, \end{aligned} \quad (4.30)$$

so the balance equations assume the following form

$$\begin{aligned} \frac{d\rho}{dt} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\ \rho \frac{dv_i}{dt} + \frac{\partial}{\partial x_i} [p + \alpha_0] + \frac{\partial \rho_{<ij>}}{\partial x_k} &= \rho f_i, \\ 3\rho \frac{d\theta}{dt} + 2 \frac{\partial q_k}{\partial x_k} + 2(p + \alpha_0) \frac{\partial v_k}{\partial x_k} + \\ + 2\rho_{<lk>} \frac{\partial v_l}{\partial x_k} &= 3A_0, \end{aligned} \quad (4.31)$$

with the balance equations for the stress tensor and heat flux,

$$\begin{aligned} \frac{d\rho_{<ij>}}{dt} + \frac{4}{5} \frac{\partial q_j}{\partial x_{<i}} + \rho_{<ij>} \frac{\partial v_k}{\partial x_k} + 2(p + \alpha_0) \frac{\partial v_{<i}}{\partial x_j} + 2\rho_{k<i}}{\partial x_k} \frac{\partial v_j}{\partial x_k} &= A_1 \rho_{<ij>}, \\ 2 \frac{dq_i}{dt} + \frac{\partial}{\partial x_i} [5\rho\theta^2 + \gamma_0] + \frac{\partial}{\partial x_k} [7\theta\rho_{<ik>}] + \\ + \frac{4}{5} \left[q_i \frac{\partial v_k}{\partial x_k} + q_l \frac{\partial v_l}{\partial x_i} + \frac{7}{2} q_k \frac{\partial v_i}{\partial x_k} \right] + 2q_i \frac{\partial v_k}{\partial x_k} + \\ - \left[2 \frac{\rho_{<il>}}{\rho} + 5 \frac{\rho\theta_{il}}{\rho} \right] \left[\frac{\partial}{\partial x_l} (p + \alpha_0) + \frac{\partial \rho_{<lk>}}{\partial x_k} \right] &= B_1 q_i. \end{aligned} \quad (4.32)$$

By insertion of this 0th order terms α_0 and γ_0 that are peculiar of moderate dense gases, we obtain a closed system of the balance equations for the 13 moments ρ , θ , v_i , $\rho_{<ij>}$ and q_i .

With these quantities the second Maxwellian iteration (4.28) assumes the form

$$\begin{aligned} 2(\rho\theta + \alpha_0) \frac{\partial v_{<i}}{\partial x_j} &= -|A_1| \rho_{<ij>}, \\ \left[5\rho\theta + \frac{\partial \gamma_0}{\partial \theta} - 5\theta \frac{\partial \alpha_0}{\partial \theta} \right] \frac{\partial \theta}{\partial x_i} + \left[\frac{\partial \gamma_0}{\partial \rho} - 5\theta \frac{\partial \alpha_0}{\partial \rho} \right] \frac{\partial \rho}{\partial x_i} &= -|B_1| q_i. \end{aligned} \quad (4.33)$$

We obtain a generalization of the viscosity coefficient μ , that becomes

$$\mu = \frac{\rho\theta + \alpha_0}{|A_1|} = \frac{\rho\theta + \frac{(1+e)\pi g_0 \rho^2 \theta d_p^3}{3m}}{4(1+e)(3-e)g_0 \sqrt{\pi\theta} \rho d_p^2 \frac{5m}}{5m}} \quad (4.34)$$

and a modified heat conductivity

$$k = \frac{5\rho\theta + \frac{\partial \gamma_0}{\partial \theta} - 5\theta \frac{\partial \alpha_0}{\partial \theta}}{|B_1|}. \quad (4.35)$$

As in [Jenkins and Richman, 1985a] we have also a dependence of the heat flux on the density gradient.

It was not possible to evaluate the coefficients of the terms of higher order in (4.19) by comparison with the results obtained with the Grad theory for the presence of the terms with the divergence of the velocity field.

4.6 Concluding remarks and perspective

A quasi linear model of 13 balance equations for 13 moments was derived for moderately dense and granular gases in the context of Extended Thermodynamics. The fluxes and the source terms were determined by expressing them as linear expressions with respect to the terms of the non equilibrium ρ_{ij} and q_i . Then through the Maxwellian iteration made up to the first order, the bulk viscosity and the thermal

conductivity were respectively determined by comparison with the laws of Navier Stokes and Fourier. It would be interesting as a future perspective to extend the model to the case of granular and dense gases with more than 13 moments.

Chapter 5

An Extended Thermodynamic Model for blood flow

5.1 Introduction

In 2009 Gidaspow and Huang [Gidaspow and Huang, 2009] idealized a biphasic blood model, consisting of plasma and red blood cells to study the behavior of blood in narrow vessels. Their model describes the Fahraeus-Lindqvist effect, which is the migration of red blood cells from the wall to the center of vessels due to a thermal gradient. Various models for blood flow were then developed to study physiological and clinical cases. For example in [Huang, Lyczkowski, and Gidaspow, 2009] the pulsing flow in a coronary artery is studied. The change in rheology of red blood cells determined by infectious diseases, environmental and hereditary factors is investigated in [Fedosov et al., 2014]. The detection and the treatment of tumors by recognizing tumor markers on the blood cell surfaces is numerically treated in [Felicetti et al., 2014]. In [Wu et al., 2015] blood flow in several benchmark microchannels is studied using a two-fluid approach. The blood flow in carotid vessels is described in [Lopes et al., 2019] and the effects of platelets are investigated in [Gidaspow and Chandra, 2014].

Recently, we introduced a biphasic model [Barbera and Pollino, 2022] in the context of Extended Thermodynamics [Müller and Ruggeri, 2013; Ruggeri and Sugiyama, 2015] that generalizes Gidaspow's results [Gidaspow and Huang, 2009] on blood flow and gives more detailed information on heat flow and the stress tensor of red blood cells. In this chapter we incorporate the white blood cells to our previous model [Barbera and Pollino, 2022]. Therefore, we define a three phasic model, consisting of plasma, red and white blood cells, aimed to investigate the variation in density and velocity of red and white blood cells in narrow blood vessels.

In particular, following the ideas of Extended Thermodynamics (ET), we consider as field variables not only the classical ones (density, velocity and temperature) but also the stress tensor, the dynamic pressure and the heat flux. The field equations are balance laws, closed by local and instantaneous constitutive relations, which are obtained using physical universal laws, like the Galilean and the entropy principles. The obtained model is hyperbolic. Hyperbolicity guarantees finite speeds of propagation and hyperbolic models are better suited to describe transient regimes.

The production terms are obtained by comparison of our model with [Gidaspow and Huang, 2009] and in particular using physical parameters, such as the viscosity and heat conductivity determined in [Gidaspow, 1994] in the context of the kinetic theory. In this way our model coincide with the classical one [Gidaspow and Huang, 2009] when the white blood cells are neglected and we are in presence of slowly changing fields and small gradients.

On the contrary, our model can describe processes where rapid time changes or when a strong deviation from equilibrium occur. In fact, it has been shown that the field equations of ET can describe a range various non-equilibrium phenomena such as light shattering, sound waves, heat waves, structure of shock waves [Müller and Ruggeri, 2013; Ruggeri and Sugiyama, 2021]. ET has been applied, with many interesting results, to monatomic gases [Müller and Ruggeri, 2013] and mixtures [Müller and Ruggeri, 2013; Kremer and Marques Jr, 2011], showing in particular the possibility to describe the thermal-diffusion effect. Recently, ET has been generalized to dense and rarefied polyatomic gases both in the classical [Ruggeri and Sugiyama, 2021] and in the relativistic framework, metal electrons and biological models, heat transfer in different symmetries and gas bubbles providing in all cases relevant results.

5.2 Balance Equations

In this section we introduce a 3-phase model consisting of plasma, red blood and white blood cells, which generalizes the 2-phase model obtained in [Barbera and Pollino, 2022]. The aim is to investigate the differences in density and velocity between red blood and white blood cells, when an energy gradient between the walls and the center of narrow blood vessels is applied. As already said, the present model is obtained in the context of ET [Müller and Ruggeri, 2013; Ruggeri and Sugiyama, 2021] so, in line with this theory, we consider the density, the velocity, the temperature, the stress tensor and the heat flux as field variables. Furthermore, in agreement with the mixture approach [Müller and Ruggeri, 2013; Ruggeri and Sugiyama, 2015; Kremer and Marques Jr, 2011], we introduce the conservation laws of mass, momentum and total energy, and the balance laws for the stress tensor and for the heat flux appropriate to each phase ($\alpha = f, r, w$). Therefore, the system of balance equations assumes the following form:

$$\begin{aligned}
\frac{\partial \rho^\alpha}{\partial t} + \frac{\partial (\rho^\alpha v_k^\alpha)}{\partial x_k} &= 0, \\
\frac{\partial (\rho^\alpha v_i^\alpha)}{\partial t} + \frac{\partial F_{ik}^\alpha}{\partial x_k} &= \rho^\alpha g_i + I_i^\alpha = H_i^\alpha, \\
\frac{\partial M_{il}^\alpha}{\partial t} + \frac{\partial M_{kll}^\alpha}{\partial x_k} &= 2v_l^\alpha H_l^\alpha + 2I^\alpha, \\
\frac{\partial F_{ij}^\alpha}{\partial t} + \frac{\partial F_{ijk}^\alpha}{\partial x_k} &= 2v_{(i}^\alpha H_{j)}^\alpha + S_{ij}^\alpha, \\
\frac{\partial M_{ill}^\alpha}{\partial t} + \frac{\partial M_{ikll}^\alpha}{\partial x_k} &= 3v_{(i}^\alpha v_l^\alpha H_l^\alpha + 2\frac{\rho_{il}^\alpha}{\rho^\alpha} H_l^\alpha + 2e^\alpha H_i^\alpha + 2v_i^\alpha I^\alpha + S_{ill}^\alpha.
\end{aligned} \tag{5.1}$$

The round brackets in the indexes indicate symmetric part, ρ^α is the density, v_k^α the velocity, F_{ik}^α the momentum, M_{il}^α the total energy, M_{kll}^α the energy flux, F_{ijk}^α the flux of momentum F_{ij}^α , while M_{ikll}^α is the flux of M_{ill}^α for the α -component. The terms in the right-hand-side represent the external forces, g_i is the external specific force, the interactions, I_i^α and I^α , and the productions S^α . In particular

$$I_i^\alpha = \sum_{\gamma \neq \alpha} \psi_{\gamma\alpha} (v_i^\gamma - v_i^\alpha), \tag{5.2}$$

where the coefficient ψ_{rf} is determined by Gidaspow in [Gidaspow and Huang, 2009; Gidaspow, 1994]. The others will be introduced later.

Experimental values

Tube diameter	0.19mm
Plasma density	1020Kgm ⁻³
Plasma viscosity	0.0012Kgm ⁻¹ s ⁻¹
RBC size	8μm
GBC size	9μm
RBC density	1092Kgm ⁻³
GBC density	1080Kgm ⁻³
Restitution coefficient	0.95

It is easy to see that system (5.1) for each constituent has the typical form of polyatomic gases, see [Ruggeri and Sugiyama, 2021] where the double hierarchies of equations was introduced.

The whole system consists of a not-closed set of field equations. In the following section we close this set of equations by use of physical universal principles and we will express all quantities in terms of the field variables through constitutive functions.

5.3 Constitutive relations

We start requiring the validity of Galilean invariance principle: the balance laws must hold in every inertial frame, so they must be invariant under a Galilean transformation. This implies the velocity dependence of densities, fluxes and productions, i.e.

$$\begin{aligned}
F_{ik}^\alpha &= \rho_{ik}^\alpha + \rho^\alpha v_i^\alpha v_k^\alpha, \\
F_{ijk}^\alpha &= \rho_{ijk}^\alpha + 3\rho_{(ij}^\alpha v_{k)}^\alpha + \rho^\alpha v_i^\alpha v_j^\alpha v_k^\alpha, \\
M_{il}^\alpha &= 2\rho^\alpha e^\alpha + \rho^\alpha v_l^\alpha v_l^\alpha, \\
M_{ill}^\alpha &= 2q_i^\alpha + 2\rho_{il}^\alpha v_l^\alpha + 2\rho^\alpha e^\alpha v_i^\alpha + \rho^\alpha v_l^\alpha v_l^\alpha v_i^\alpha, \\
M_{ikll}^\alpha &= m_{ikll}^\alpha + 2\rho_{ikl}^\alpha v_l^\alpha + 4q_{(i}^\alpha v_{k)}^\alpha + 4\rho_{l(i}^\alpha v_{k)}^\alpha v_l^\alpha + \\
&\quad + \rho_{ik}^\alpha v_l^\alpha v_l^\alpha + 2\rho^\alpha e^\alpha v_i^\alpha v_k^\alpha + \rho^\alpha v_i^\alpha v_k^\alpha v_l^\alpha v_l^\alpha, \\
S_{ij}^\alpha &= s_{ij}^\alpha, \\
S_{ill}^\alpha &= s_{ill}^\alpha + 2v_l^\alpha s_{ij}^\alpha,
\end{aligned} \tag{5.3}$$

where ρ_{ik}^α is the stress tensor, $e^\alpha = 3\theta^\alpha$ the specific internal energy, θ^α the temperature and q_i^α the heat flux. The quantities ρ_{ik}^α , ρ_{ijk}^α , $2\rho^\alpha e^\alpha$, $2q_i^\alpha$, m_{ikll}^α , s_{ij}^α and s_{ill}^α are the internal quantities that are independent on the velocity fields. We observe that a simpler method for obtaining Galilean invariance is present in [Pennisi and Ruggeri, 2006]. So, as a result of the principle of Galilean invariance for each component, the field

equations can be written in a particular form

$$\begin{aligned}
\frac{d_\alpha \rho^\alpha}{dt} + \rho^\alpha \frac{\partial v_k^\alpha}{\partial x_k} &= 0, \\
\rho^\alpha \frac{d_\alpha v_i^\alpha}{dt} + \frac{\partial \rho_{ik}^\alpha}{\partial x_k} &= H_i^\alpha, \\
3 \frac{d_\alpha}{dt} (\rho^\alpha \theta^\alpha) + 3 \rho^\alpha \theta^\alpha \frac{\partial v_k^\alpha}{\partial x_k} + \rho_{kl}^\alpha \frac{\partial v_l^\alpha}{\partial x_k} + \frac{\partial q_k^\alpha}{\partial x_k} &= I^\alpha, \\
\frac{d_\alpha \rho_{ij}^\alpha}{dt} + \rho_{ij}^\alpha \frac{\partial v_k^\alpha}{\partial x_k} + 2 \rho_{k(i}^\alpha \frac{\partial v_{j)}^\alpha}{\partial x_k} + \frac{\partial \rho_{kij}^\alpha}{\partial x_k} &= S_{ij}^\alpha, \\
2 \frac{d_\alpha q_i^\alpha}{dt} + \frac{\partial m_{ikll}^\alpha}{\partial x_k} + 2 \rho_{ikl}^\alpha \frac{\partial v_l^\alpha}{\partial x_k} + 4 q_i^\alpha \frac{\partial v_k^\alpha}{\partial x_k} - 2 \frac{\rho_{il}^\alpha}{\rho^\alpha} \frac{\partial \rho_{lk}^\alpha}{\partial x_k} - 6 \theta^\alpha \frac{\partial \rho_{ik}^\alpha}{\partial x_k} &= s_{ill}^\alpha,
\end{aligned} \tag{5.4}$$

where $d_\alpha/dt = \partial/\partial t + v_k^\alpha \partial/\partial x_k$ are the material derivatives.

We further decompose the stress tensors for the blood cells and plasma as the sum of their traceless and trace parts:

$$\begin{aligned}
\rho_{ik}^\beta &= \rho_{\langle ik \rangle}^\beta + (p^\beta + \Delta^\beta) \delta_{ik}, \quad \text{with } \beta = r, w, \\
\rho_{ik}^f &= \rho_{\langle ik \rangle}^f + p^f \delta_{ik},
\end{aligned} \tag{5.5}$$

where¹ the angular brackets indicate the traceless part of a tensor.

We consider $\rho_{\langle ik \rangle}^\alpha$ and Δ^β as field variables instead of ρ_{ik}^α , while the pressures p^α must be expressed in terms of the fields though the respective thermal equations of state. Furthermore, according to the principle of material indifference for the whole mixture [Kremer and Marques Jr, 2011], the fields cannot depend on the velocity v_k^α separately, but on the diffusion velocity u_i^α and the blood velocity v_i :

$$u_i^\alpha = v_i^\alpha - v_i \quad \text{and} \quad v_i = \frac{\rho^r v_i^r + \rho^w v_i^w + \rho^f v_i^f}{\rho^r + \rho^w + \rho^f}. \tag{5.6}$$

Therefore, set (5.4) is a system of 41 equations for the 41 field variables: densities ρ^α , diffusion velocities u_i^r, u_i^s , blood velocity v_i , temperatures θ^α , traceless parts of the stress tensors $\rho_{\langle ij \rangle}^\alpha$, dynamic pressures Δ^β and heat fluxes q_i^α .

The remaining unknowns $\rho_{ijk}^\alpha, m_{ikll}^\alpha, s_{ij}^\alpha$ and s_{ill}^α in (5.4) must be determined explicitly in terms of $\rho^\alpha, \theta^\alpha, \rho_{\langle ij \rangle}^\alpha, \Delta^\beta, q_i^\alpha$ through constitutive functions. In line with ET, we assume that these functions are local and instantaneous so, at one time and at one position, they must depend on the fields at the same time and position.

We demand the validity of the entropy principle that assumes the existence of a concave entropy density h , an entropy flux $h_k = h v_k + \phi_k$ and an entropy production Φ that satisfy a balance equation of the form

$$\frac{\partial h}{\partial t} + \frac{\partial h_k}{\partial x_k} = \Phi \geq 0 \tag{5.7}$$

for all thermodynamic processes, that is for all solutions of the field equations.

The entropy principle can be mathematically evaluated by use of the Liu-Lagrange multipliers λ . In fact the balance equations (5.4) are considered as constrains for the

¹Throughout the chapter, β is used when only red and white blood cells are considered.

validity of the entropy inequality (5.7). Therefore relation

$$\begin{aligned}
& \frac{\partial h}{\partial t} + \frac{\partial(hv_k + \phi_k)}{\partial x_k} - \sum_{\alpha=r,w,f} \left\{ \lambda^\alpha \left[\frac{d_\alpha \rho^\alpha}{dt} + \rho^\alpha \frac{\partial v_k^\alpha}{\partial x_k} \right] + \right. \\
& + \frac{1}{\rho^\alpha} (\rho^\alpha \lambda_i^\alpha - 2\rho_{ik}^\alpha \lambda_{km}^\alpha - 3\rho^\alpha \theta^\alpha \lambda_{inn}^\alpha) \left[\rho^\alpha \frac{d_\alpha v_i^\alpha}{dt} + \frac{\partial \rho_{ik}^\alpha}{\partial x_k} - H_i^\alpha \right] \\
& + \hat{\lambda}_{ll}^\alpha \left[\frac{d_\alpha}{dt} (\rho^\alpha e^\alpha) + \rho^\alpha e^\alpha \frac{\partial v_k^\alpha}{\partial x_k} + \rho_{kl}^\alpha \frac{\partial v_l^\alpha}{\partial x_k} + \frac{\partial q_k^\alpha}{\partial x_k} - I^\alpha \right] + \\
& + \lambda_{ij}^\alpha \left[\frac{d_\alpha \rho_{ij}^\alpha}{dt} + \rho_{ij}^\alpha \frac{\partial v_k^\alpha}{\partial x_k} + 2\rho_{k(i}^\alpha \frac{\partial v_{j)}^\alpha}{\partial x_k} + \frac{\partial \rho_{kij}^\alpha}{\partial x_k} - s_{ij}^\alpha \right] + \\
& \left. + \lambda_{inn}^\alpha \left[2 \frac{d_\alpha q_i^\alpha}{dt} + \frac{\partial m_{ikll}^\alpha}{\partial x_k} + 2\rho_{ikl}^\alpha \frac{\partial v_l^\alpha}{\partial x_k} + 4q_{(i}^\alpha \frac{\partial v_{k)}^\alpha}{\partial x_k} - 2 \frac{\rho_{il}^\alpha}{\rho^\alpha} \frac{\partial \rho_{lk}^\alpha}{\partial x_k} - 2e^\alpha \frac{\partial \rho_{lk}^\alpha}{\partial x_k} - s_{ill}^\alpha \right] \right\} = \Phi
\end{aligned} \tag{5.8}$$

must be valid for all $\rho^\alpha, \theta^\alpha, u_i^\beta, v_i, \rho_{<ij>}^\alpha, \Delta^\beta, q_i^\alpha$.

Clearly, also the entropy density h , the entropy flux ϕ_k the entropy production Φ and the Lagrange multipliers must be expressed in terms of the fields by constitutive functions. Then equation (5.8) is evaluated setting the coefficients of the field variables and their derivatives equal to zero.

Since our aim is to focus on processes close to thermodynamic equilibrium, in order to simplify the calculations, we expand the constitutive functions, the Lagrange and the entropic quantities in terms of the non-equilibrium fluxes $\rho_{<ij>}^\alpha, \Delta^\beta$ and q_i^α . In particular, the constitutive relations are

$$\begin{aligned}
\rho_{ijk}^\alpha &= 3\eta^\alpha q_{(i}^\alpha \delta_{jk)} + O(2), \\
m_{ijll}^\beta &= \gamma_1^\beta \rho_{<ij>}^\beta + \frac{1}{3} [\gamma_0^\beta + \gamma_2^\beta \Delta^\beta] \delta_{ij} + O(2), \\
m_{ijll}^f &= \gamma_1^f \rho_{<ij>}^f + \frac{1}{3} \gamma_0^f \delta_{ij} + O(2),
\end{aligned} \tag{5.9}$$

where the coefficients depends only on the equilibrium variables ($\rho^\alpha, \theta^\alpha$). Analogous expansions are considered for the entropy quantities and the Lagrange multipliers but the entropy quantities are expanded till the second order terms in order to have a coherent evaluation of (5.8). So, inserting all expansions into the entropy equation (5.8) and equating all coefficients of the field derivatives to zero, we can find out, after some long calculations, the expression of the functions in (5.9) as follows:

$$\begin{aligned}
\eta^\alpha &= \frac{p^\alpha \theta^\alpha}{\Psi^\alpha} \left[\gamma_1^\alpha - 2 \left(\frac{p^\alpha}{\rho^\alpha} + e^\alpha \right) \right], \\
\frac{\partial \gamma_0^\alpha}{\partial \rho^\alpha} &= 6 \left(e^\alpha + \frac{p^\alpha}{\rho^\alpha} \right) p_\rho^\alpha, \\
\frac{\partial}{\partial \rho^\alpha} [p^\alpha \gamma_1^\alpha] &= 2 \left[2 \frac{p^\alpha}{\rho^\alpha} + e^\alpha \right] p_\rho^\alpha, \\
\gamma_2^\beta &= -\frac{3}{\Gamma^\beta} \left[\frac{5}{3} p^\beta \gamma_1^\beta - 2 \left(e^\beta + \frac{p^\beta}{\rho^\beta} \right) (\Gamma^\beta + \frac{5}{3} p^\beta) + \frac{\Psi^\beta p_\theta^\beta}{\rho^\beta c_V^\beta \theta^\beta} \right],
\end{aligned} \tag{5.10}$$

where

$$\begin{aligned}
\Psi^\beta &= -\frac{\theta_2^\beta}{3} \frac{\partial \gamma_0^\beta}{\partial \theta^\beta} + 2\theta_2^\beta \left(e^\beta + \frac{p^\beta}{\rho^\beta} \right) p_\theta^\beta, \\
\Gamma^\beta &= -\frac{5}{3} p^\beta + \rho^\beta p_\rho^\beta + \frac{\theta^\beta (p_\theta^\beta)^2}{\rho^\beta c_V^\beta}.
\end{aligned} \tag{5.11}$$

We use the expression of the pressure for red blood cells, determined by Gidaspow [Gidaspow, 1994; Gidaspow and Huang, 2009] and we assume a similar dependence for the white blood cells

$$p_\beta = (1 + 2\chi_\beta) \rho_\beta \theta_\beta \quad \text{with} \quad \chi_\beta = (1 + e) \epsilon_\beta g_0^\beta, \quad (5.12)$$

where ϵ_α is the phase volume fraction, g_0^β the radial distribution function and e is the restitution coefficient, a measure of the elasticity of the collisions between cells. Using these pressures, the constituent relations (5.10) take the more manageable form

$$\begin{aligned} \gamma_0^\beta &= 12 (2 + \chi_\beta) (1 + 2\chi_\beta) \rho_\beta \theta_\beta^2, \\ \gamma_1^\beta &= 2 (5 + 4\chi_\beta) \theta_\beta, \\ \gamma_2^\beta &= 6 (5 + 4\chi_\beta) \theta_\beta, \\ \eta^\beta &= \frac{1}{2} \frac{1+2\chi_\beta}{2+\chi_\beta}. \end{aligned} \quad (5.13)$$

In conclusion, the left-hand sides of the balance equations (5.4) with relations (5.5, 5.9-5.13), are explicitly expressed in terms of the field variables. In the next section we will instead evaluate the right-hand side of these equations.

5.4 Production terms

Following the BGK hypothesis, we assume each production term proportional to the corresponding density minus its equilibrium value, that is

$$s_{<ij>}^\alpha = -\frac{\rho_{<ij>}^\alpha}{\tau_\sigma^\alpha}, \quad s_{ll}^\beta = -3\frac{\Delta^\beta}{\tau_\Delta^\beta}, \quad s_{ill}^\alpha = -2\frac{q_l^\alpha}{\tau_q^\alpha}. \quad (5.14)$$

The coefficients τ are the relaxation times which must be determined in terms of the equilibrium variables. Here we evaluate them by comparison of our equations with the corresponding classical ones in [Gidaspow and Huang, 2009; Gidaspow, 1994]. This comparison can be done through the so-called Maxwellian iterations (see for example [Müller and Ruggeri, 2013]: We insert the productions (5.14) into the balance equations (5.4)_{4,5} and we neglect all non-equilibrium terms in the left-hand-side of these equations. The relations so determined find a perfect analogy with the Navier-Stokes and the Fourier equations for the stress tensor and the heat flux, respectively. In fact we have

$$\begin{aligned} 2p^\alpha \frac{\partial v_{<i>}^\alpha}{\partial x_{j>}} &= -\frac{\rho_{<ij>}^\alpha}{\tau_\sigma^\alpha}, \\ \frac{5}{3} p^\beta \frac{\partial v_k^\beta}{\partial x_k} &= -\frac{\Delta^\beta}{\tau_\Delta^\beta}, \\ \left[\frac{1}{3} \frac{\partial \gamma_0^\alpha}{\partial \theta_\alpha} - 2 \left(\frac{p_\alpha}{\rho_\alpha} + 3\theta_\alpha \right) \frac{\partial p_\alpha}{\partial \theta_\alpha} \right] \frac{\partial \theta_\alpha}{\partial x_k} &= -2 \frac{q_k^\alpha}{\tau_q^\alpha}. \end{aligned} \quad (5.15)$$

In this way the relaxation times can be evaluated using the shear viscosity, bulk viscosity and heat conductivity calculated for red blood cells in [gidaspow ; Gidaspow, 1994]. We assume that these expressions are valid also for white blood cells with

appropriate values for the coefficients. Then we have

$$\begin{aligned}
\tau_\sigma^\beta &= \frac{1}{1+2\chi_\beta} \left[\frac{4}{5} + \frac{10}{96} \frac{\pi\epsilon_\beta}{\chi_\beta^2} \left(1 + \frac{4}{5}\chi_\beta\right)^2 \right] \frac{\chi_\beta d_p^\beta}{\sqrt{\pi\theta_\beta}}, \\
\tau_\sigma^f &= \epsilon_f \frac{\mu_f}{p_f}, \\
\tau_\Delta^\beta &= \frac{4}{5} \frac{1}{1+2\chi_\beta} \frac{\chi_\beta d_p^\beta}{\sqrt{\pi\theta_\beta}}, \\
\tau_q^\beta &= \frac{1}{(1+2\chi_\beta)(2+\chi_\beta)} \left[1 + \frac{75}{384} \frac{\pi\epsilon_\beta}{\chi_\beta^2} \left(1 + \frac{6}{5}\chi_\beta\right)^2 \right] \frac{\chi_\beta d_p^\beta}{\sqrt{\pi\theta_\beta}}, \\
\tau_q^f &= \kappa_f \left[\frac{1}{6} \frac{\partial \gamma_0^f}{\partial \theta_f} - \left(\frac{p_f}{\rho_f} + 3\theta_f \right) \frac{\partial p_f}{\partial \theta_f} \right]^{-1},
\end{aligned} \tag{5.16}$$

where d_p^β is the diameter of red and white blood cells, $\epsilon_f \mu_f$ and κ_f are the viscosity and heat conductivity of plasma.

The interaction terms in the balance laws of momentum and energy are evaluated through the values determined by Savage et al [Savage, 1983], which takes into account the inelastic collision of particles

$$I^\beta = -\frac{12(1-e^2)g_0^\beta}{d_p^\beta \sqrt{\pi}} \rho_\beta \epsilon_\beta \theta_\beta^{\frac{3}{2}} \quad \text{and} \quad I^f = -I^r - I^w. \tag{5.17}$$

Finally, the coefficients ψ_{fr} and ψ_{fw} in (5.2), taking into account the interactions between plasma and red or white blood cells respectively, are given by

$$\psi_{f\beta} = \begin{cases} \frac{150\epsilon_\beta^2 \mu_f}{(1-\epsilon_\beta)d_{p\beta}^2} & \text{if } \epsilon_f \leq 0.8, \\ 0 & \text{if } \epsilon_f > 0.8, \end{cases} \tag{5.18}$$

(see Gidaspow (2009)) and we assume that coefficient ψ_{rw} in (5.2), which expresses the interactions between red and white blood cells, is constant.

Substitution of (5.2,5.14,5.16-5.18) into balance equations (5.4) makes also the right-hand side completely explicit in terms of the fields. Therefore, equations (5.4) with the constitutive relations (5.2,5.5,5.14-5.18) form a closed set of 41 field equations in the 41 fields ρ^α , u_i^β , v_i , θ^α , $\rho_{<ij>}^\alpha$, Δ^β and q_i^α .

5.5 Planar analytical solutions

We study now the blood flow in a narrow vessel idealized as the gap between two infinite parallel plates. We assume that the fields ρ^α , θ^α , $\rho_{<ij>}^\alpha$, Δ^β , q_i^α and v_i^α depend only on the $x_1 = x$ orthogonal to the two plates and $v_i^\alpha = (0, 0, v_z^\alpha)$, where $x_3 = z$ lies the direction of the flow.

In order to solve easily the problem, we linearize the field equations around the constant equilibrium solution $(\rho_0^\alpha, \theta_0)$ and introduce the following dimensionless quantities

$$\begin{aligned}
\hat{x} &= \frac{x}{L}, & \hat{\theta}^\alpha &= \frac{\theta^\alpha}{\theta_0}, & \hat{p}^\alpha &= \frac{p^\alpha}{\rho_0^\alpha \theta_0}, & \hat{\rho}_{<ij>}^\alpha &= \frac{\rho_{<ij>}^\alpha}{\rho_0^\alpha \theta_0}, \\
\hat{\Delta}^\beta &= \frac{\Delta^\beta}{\rho_0^\beta \theta_0}, & \hat{v}_z^\alpha &= \frac{v_z^\alpha}{\sqrt{\theta_0}}, & \hat{q}_i^\alpha &= \frac{q_i^\alpha}{\rho_0^\alpha \theta_0 \sqrt{\theta_0}}.
\end{aligned} \tag{5.19}$$

L is the distance between the two plates. With some simple calculations, the linearized model assumes the following form

$$\begin{aligned}
\frac{d\hat{p}^\alpha}{d\hat{x}} &= 0, \\
\frac{d\hat{\rho}_{<13>}^\alpha}{d\hat{x}} &= \hat{g} + \sum_\gamma \hat{\psi}_{\gamma\alpha} (\hat{\theta}_3^\gamma - \hat{\theta}_3^\alpha), \\
\frac{d\hat{q}_1^\alpha}{d\hat{x}} &= \hat{I}^\alpha, \\
\hat{\rho}_{<11>}^\alpha &= -2\hat{\rho}_{<33>}^\alpha = -\frac{4}{3}\hat{\tau}_\sigma^\alpha \eta^\alpha \hat{I}^\alpha, \\
\hat{\Delta}^\beta &= -\frac{5}{3}\hat{\tau}_\Delta^\beta \eta^\beta \hat{I}^\beta, \\
\hat{p}_0^\alpha \frac{d\hat{\theta}_3^\alpha}{d\hat{x}} + \eta^\alpha \frac{d\hat{q}_3^\alpha}{d\hat{x}} &= -\frac{\hat{\rho}_{<13>}^\alpha}{\hat{\tau}_\sigma^\alpha}, \\
\frac{1}{6}\hat{\gamma}_0^\alpha \frac{d\hat{\theta}^\alpha}{d\hat{x}} &= -\frac{\hat{q}_1^\alpha}{\hat{\tau}_q^\alpha}, \\
\frac{1}{2} \left[\hat{\gamma}_1^\alpha - 2 \left(\frac{p_0^\alpha}{\rho_0^\alpha} + 3\theta \right) \right] \frac{d\hat{\rho}_{<13>}^\alpha}{d\hat{x}} &= -\frac{\hat{q}_3^\alpha}{\hat{\tau}_q^\alpha}
\end{aligned} \tag{5.20}$$

with the dimensionless functions for the red and white blood cells given by

$$\begin{aligned}
\hat{\gamma}_0^\beta &= 12 (2 + \chi_\beta) (1 + 2\chi_\beta), \\
\hat{\gamma}_1^\beta &= 2 (5 + 4\chi_\beta).
\end{aligned} \tag{5.21}$$

If we assume that plasma behaves as a perfect fluid, we also have

$$\hat{\gamma}_0^f = 24, \quad \text{and} \quad \hat{\gamma}_1^f = 10. \tag{5.22}$$

The dimensionless terms related to the productions are instead

$$\hat{g} = \frac{g_3 L}{\theta_0}, \quad \hat{\psi}_{\gamma\alpha} = \frac{\psi_{\gamma\alpha} L}{\rho_0^\alpha \sqrt{\theta_0}}, \quad \hat{I}^\alpha = \frac{I^\alpha L}{\rho_0^\alpha \sqrt{\theta_0}}, \quad \hat{\tau}^\alpha = \frac{\tau^\alpha L}{\sqrt{\theta_0}}. \tag{5.23}$$

It can be easily seen that equations (5.20)_{4,5} are algebraic and combination of (5.20)_{2,8} furnishes algebraic relations for \hat{q}_3^α in terms of the velocity fields. Therefore, the whole set (5.20) consists of a system of ODEs of order 15. This system can be analytically integrated assuming that the three blood constituents have the temperature θ_0 and vanishing velocities at both boundaries, that coincide with the vessel walls, and prescribing their pressures at one boundary P^α . In this way, we have the 15 boundary conditions that we need for the determination of the 15 integration constants.

Integrating equations (5.20)_{1,3,7} we easily get

$$\hat{p}^\alpha = P^\alpha, \quad \hat{q}_1^\alpha = \hat{I}^\alpha \hat{x}, \quad \hat{\theta}^\alpha = -\frac{3\hat{I}^\alpha}{\hat{\gamma}_0^\alpha \hat{\tau}_q^\alpha} \left(\hat{x}^2 - \frac{1}{4} \right) + 1. \tag{5.24}$$

These solutions obtained with the values of the parameters $\varepsilon_r = 0.4$ and $\varepsilon_w = 0.01$ are illustrated in Fig.1. As it can be easily seen, the two temperatures decrease at the center of the vessel where instead both densities reach their maximum value. This result is in agreement with the Fahraeus-Lindqvist effect, indeed the experimental results predict that the red blood cells in small vessel concentrate in the center of the channel. From Fig.1b, it can be easily seen that also the white blood cells concentrate at the center, but this behavior is more evident, since white blood cells constitute a very small fraction (less than 1%) of total blood volume.

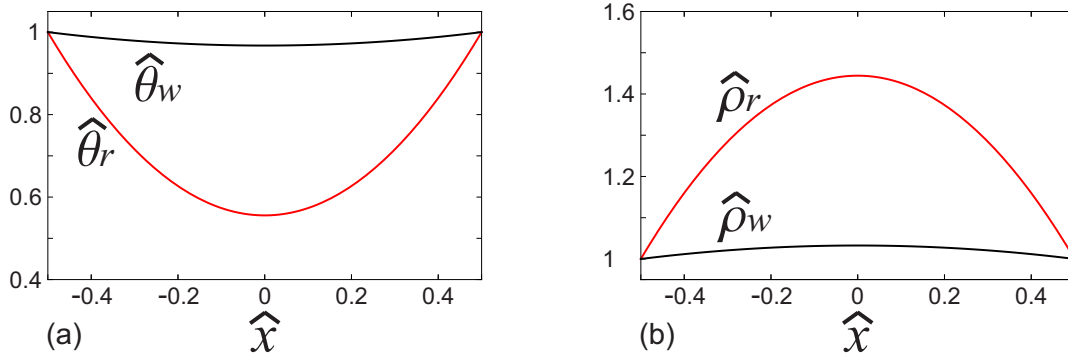


FIGURE 5.1: Dimensionless red and white blood cells temperatures (Fig.1a) and dimensionless densities (Fig.1b). The graphs are obtained with the values in Table 1, $\varepsilon_r = 0.4$ and $\varepsilon_w = 0.01$.

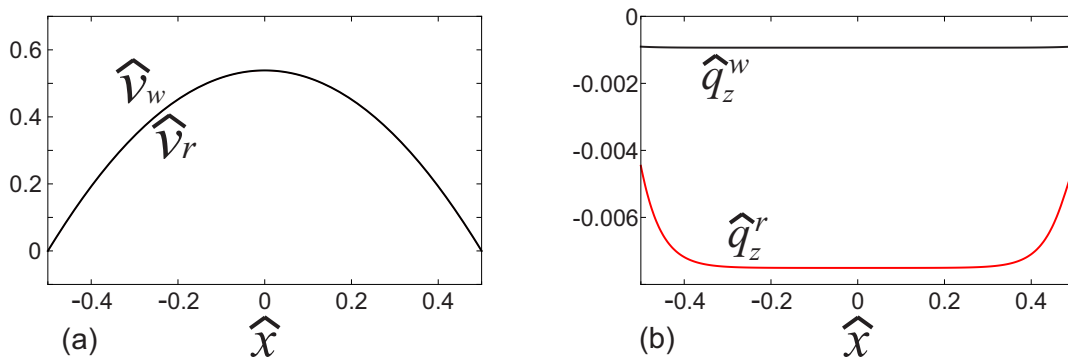


FIGURE 5.2: Dimensionless red and white blood cells velocities (Fig.2a) and heat flux in the direction of the flow (Fig.2b). The graphs are obtained with the values in Table 1, $\varepsilon_r = 0.4$ and $\varepsilon_w = 0.01$.

Also the remaining equations (5.20)_{2,6,8} can be analytically integrated but the solution assumes a too complicate form to be written here due to the combinations of the three velocities in (5.20)₂. For this reason we show in this chapter only the numerical evaluation of these solutions. In particular in Fig.2 the velocity fields of both cells is illustrated. No differences between them can be observed. Finally, the solutions of the field equations (5.20) predict small but non-vanishing component of the heat flux q_z^α in the direction of the flow. This kind of solution imply a correction of the Fourier law of heat conduction and, for gases is in agreement with the kinetic theory. Also some components of the traceless parts of the stress tensor $\rho_{\langle 11 \rangle}^\alpha$ and $\rho_{\langle 22 \rangle}^\alpha$ and this solution is a correction of the Navier-Stocks laws. In addition, we also have a non-vanishing dynamic pressure for red and white blood cells.

5.6 Conclusions and Final Remarks

In this chapter we introduced a model in the context of Rational Extended Thermodynamics in order to describe the behavior of white blood cells in small vessels. The linearized field equations are integrated analytically. The solutions reveals that also the white blood cells aggregate in the center of the channel as the red ones, in agreements with the Fahraeus-Lindqvist effect. As expected, the effect of the white blood cells is small, since they constitute only a very small fraction of total blood volume,

and they do not modify the behavior of the red blood cells. It is intention of the authors to incorporate to the model also the effect of platelets.

Chapter 6

A hyperbolic reaction-diffusion model of chronic wasting disease

6.1 Introduction

Chronic wasting diseases affect several animal species, such as deer and elk, goats and sheep. Mad cow disease, which can be transmitted to humans by ingesting infected meat, is an example. These diseases are caused by misfolded proteins, called prions. Generally, prions are harmless proteins, present in nerve tissues, but when they are poorly folded, they are very dangerous because they cause deterioration of the nervous system and consequently a decline in the cognitive and motor abilities of the affected animal. It is observed that prions are transmitted to susceptible animals mainly through ingestion of soil rather than direct transmission from infected animals. So, Miller et al. [Miller, Hobbs, and Tavener, 2006] elaborated a susceptible-infected model for chronic wasting diseases in deer, where they added an environmental reservoir of the disease that can re-infect the susceptible population, instead of direct transmission from infected individuals. Sharp and Pastor [Sharp and Pastor, 2011] modified this model, replacing the constant birth rate with a logistic growth term, which is more suitable for models of diseases in wildlife populations. Barbera [Barbera, 2020] introduced the diffusion effect, taking into account the spatial dependence of the fields.

Reaction-diffusion equations are often adopted to describe dynamics of populations that interact through different mechanisms. If the diffusion effect is described by the Fick law, the model turns out to be parabolic. A drawback of parabolic model is that it provides an instantaneous relation between cause and effect which, implies the diffusion of a biological population at an infinite speed. So many authors developed various hyperbolic models by means of different mathematical approaches, see [Hillen, 2002] and the references therein.

In this chapter in order to overcome the problem, we replace parabolic equations with hyperbolic ones, using Extended Thermodynamic theory (RET) [Müller and Ruggeri, 2013] based on universal physical principles, such as the entropy principle and the principle of relativity. RET has been applied to many biological problems, such as aquatic food chains **acqua**, chemotaxis, dryland ecology, blood flow and gas bubbles with very interesting results.

Following the first model in [Barbera, 2020], in this Chapter a hyperbolic model in the context of RET able to study chronic wasting diseases caused by prions is developed. In detail, in Sect.2, the classical model is presented and the hyperbolic system is constructed. In Sect.3 the stability character of steady states is discussed analytically and in Sect.4 the numerical solutions are shown. Finally, in Sect.5 the behavior of the acceleration waves is described, which are expected to occur at finite velocity. Conclusions and remarks are present in Sect.6.

6.2 Hyperbolic model

The dynamics of wasting disease can be described through the following system of partial differential equations

$$\begin{aligned}\frac{\partial S}{\partial t} + \frac{\partial J^S}{\partial x} &= bS - \frac{S^2}{K} - \gamma SE - mS = f(S, I, E), \\ \frac{\partial I}{\partial t} + \frac{\partial J^I}{\partial x} &= \gamma SE - (m + \mu)I = g(S, I, E), \\ \frac{\partial E}{\partial t} &= \epsilon I - \tau E = h(S, I, E),\end{aligned}\tag{6.1}$$

where S and I are the number of susceptible and infected animals/100Km², and E is the quantity of infected material/100Km². The term bS represents the births of individuals, which is proportional to S . The two parameters m and μ are the mortality rates due to natural reasons ($b > m$) and to the disease, respectively. K represents the carrying capacity, typical of the logistic growth, and γ represents the probability of the disease transmission from the environment to susceptible animals via random encounter. In the last equation, ϵ is the rate by which the infected material is voided from infected animals into the soil, while τ is the loss rate of active infected material.

In system (6.1), J^S and J^I are the diffusive fluxes which, in agreement with the Fick's law, are usually assumed to be proportional to the gradient of the corresponding density, that is

$$\begin{aligned}J^S &= -D_S \frac{\partial S}{\partial x}, \\ J^I &= -D_I \frac{\partial I}{\partial x}\end{aligned}\tag{6.2}$$

with constant $D_S > 0$ and $D_I > 0$ diffusion coefficients ($D_S > D_I$).

Substitution of (6.2) into the balance equations (6.1) leads to a parabolic reaction-diffusion model based on the instantaneous diffusive effects that imply an unrealistic infinite propagation rate. Therefore, instead of assuming the Fick relations (6.2), we consider J^S and J^I as additional field variables, together with S , I and E , satisfying the following balance equations

$$\begin{aligned}\frac{\partial J^S}{\partial t} + \frac{\partial M^S}{\partial x} &= N^S, \\ \frac{\partial J^I}{\partial t} + \frac{\partial M^I}{\partial x} &= N^I.\end{aligned}\tag{6.3}$$

The fluxes M^S and M^I and the productions N^S and N^I must be determined in terms of (S, I, E, J^S, J^I) through constitutive functions. Since we are interested in processes not far from thermodynamical equilibrium, where $J^S = 0$ and $J^I = 0$, we can assume a linear dependence of these functions on the two fluxes:

$$\begin{aligned}M^S &= \varphi(S, I, E) + \varphi_1(S, I, E) J^S + \varphi_2(S, I, E) J^I, \\ M^I &= \chi(S, I, E) + \chi_1(S, I, E) J^S + \chi_2(S, I, E) J^I, \\ N^S &= v(S, I, E) + v_1(S, I, E) J^S + v_2(S, I, E) J^I, \\ N^I &= \mu(S, I, E) + \mu_1(S, I, E) J^S + \mu_2(S, I, E) J^I.\end{aligned}\tag{6.4}$$

Then, requiring that the evolution equations (6.3,6.4) reduce to the Fick laws (6.2) in the stationary case, one gets the following restrictions on (6.4):

$$\begin{aligned}M^S &= \varphi(S), \quad N^S = -\frac{\varphi'(S)}{D_S}, \\ M^I &= \chi(I), \quad N^I = -\frac{\chi'(I)}{D_I},\end{aligned}\tag{6.5}$$

where the prime stands for the derivative of the function with respect to its argument. Consequently, the evolution equations (6.3) become

$$\begin{aligned}\frac{\partial J^S}{\partial t} + \varphi'(S) \frac{\partial S}{\partial x} &= -\frac{\varphi'(S)}{D_S} J^S, \\ \frac{\partial J^I}{\partial t} + \chi'(I) \frac{\partial I}{\partial x} &= -\frac{\chi'(I)}{D_I} J^I.\end{aligned}\quad (6.6)$$

A further restriction on the constitutive quantities $\varphi'(S)$ and $\chi'(I)$ arises from the compatibility of the system (6.1,6.6) with the entropy law. Indeed the entropy principle assumes the existence of a concave entropy density η , an entropy flux ϕ and a positive entropy production Σ satisfying the balance law

$$\frac{\partial \eta}{\partial t} + \frac{\partial \phi}{\partial x} = \Sigma \geq 0 \quad (6.7)$$

for all the solutions of the field equations. In this way, the field equations (6.1,6.6) can be considered as constrains for the validity of equation (6.7). As shown in Liu, 1972, these constrains can be taken into account by using the Lagrange multipliers, Λ , Γ , X , Ω and Π . The entropy quantities and the Lagrange multipliers must be considered as constitutive functions of (S, I, E, J^S, J^I) like in (6.4). In this way, the validity of the entropy principle is ensured if

$$\begin{aligned}\eta &= \tilde{\eta}_0(S) + \hat{\eta}_0(I) + \tilde{\eta}_0(E) + \frac{\Omega_1(S)}{2} (J^S)^2 + \frac{\Pi_1(I)}{2} (J^I)^2, \\ \phi &= \Lambda_0(S) J^S + \Gamma_0(I) J^I, \\ \Lambda &= \Lambda_0(S) + \frac{\Omega'_1(S)}{2} (J^S)^2, \\ \Gamma &= \Gamma_0(I) + \frac{\Pi'_1(I)}{2} (J^I)^2, \\ X &= X_0(E), \\ \Omega &= \Omega_1(S) J^S, \\ \Pi &= \Pi_1(I) J^I\end{aligned}\quad (6.8)$$

with

$$\begin{aligned}\tilde{\eta}'_0(S) &= \Lambda_0(S), & \hat{\eta}_0(I) &= \Gamma_0(I), & \tilde{\eta}_0(E) &= \Gamma_0(E), \\ \Lambda'_0(S) &= \varphi'(S) \Omega_1(S), & \Gamma'_0(I) &= \chi'(I) \Pi_1(I)\end{aligned}\quad (6.9)$$

together with the residual inequality

$$\Sigma = \Lambda_0 f + \Gamma_0 g + X_0 h + \left(\frac{\Omega'_1 f}{2} - \frac{\Omega_1 \varphi'}{D_S} \right) (J^S)^2 - \left(\frac{\Pi'_1 f}{2} - \frac{\Pi_1 \chi'}{D_I} \right) (J^I)^2. \quad (6.10)$$

On the other hand, the concavity condition for with respect to the field variables leads to

$$\Omega_1(S) < 0, \quad \Pi_1(I) < 0, \quad \varphi'(S) > 0, \quad \chi'(I) > 0 \quad (6.11)$$

which guarantees that the relaxation times $\tau_S = D_S / \varphi'(S)$ and $\tau_I = D_I / \chi'(I)$ are positive as expected.

For further purpose, system (6.1,6.6) is recast in the following vector form

$$\mathbf{U}_t + \mathbf{A}(\mathbf{U}) \mathbf{U}_x = \mathbf{B}(\mathbf{U}), \quad (6.12)$$

where

$$\mathbf{U} = \begin{pmatrix} S \\ I \\ E \\ J^S \\ J^I \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ \varphi' & 0 & 0 & 0 & 0 \\ 0 & \chi' & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} f \\ g \\ h \\ -\frac{\varphi' J^S}{D_S} \\ -\frac{\chi' J^I}{D_I} \end{pmatrix} \quad (6.13)$$

Relations (6.11) ensure the reality of the non-vanishing characteristic speeds $\lambda_{1,2} = \pm\sqrt{\varphi'(S)}$ and $\lambda_{3,4} = \pm\sqrt{\chi'(I)}$, that are the eigenvalues of \mathbf{A} . The corresponding eigenvectors are

$$\mathbf{d}_{1,2} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \lambda_{1,2} \\ 0 \end{pmatrix} \quad \mathbf{l}_{1,2} = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{1}{\lambda_{1,2}} \\ 0 \end{pmatrix}^T \quad \mathbf{d}_{3,4} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \lambda_{3,4} \end{pmatrix} \quad \mathbf{l}_{3,4} = \frac{1}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \frac{1}{\lambda_{3,4}} \end{pmatrix}^T \quad (6.14)$$

As a consequence of the required concavity condition, the field equations (6.1,6.6) are symmetric-hyperbolic in the sense of Friedrichs and Lax **Giallo** when the Lagrange multipliers are chosen as variables and the Cauchy problem is well-posed for suitable smooth initial data.

In the particular case $\tau_S \rightarrow 0$ and $\tau_I \rightarrow 0$, the hyperbolic system (6.1,6.6) reduces to the parabolic one [Barbera, 2020].

6.3 Linear stability analysis

System (6.1,6.6) admits three spatially homogeneous equilibrium states of the form $\mathbf{U}^* = (S^*, I^*, E^*, J^{S*}, J^{I*})$, found as solutions of $\mathbf{B}(\mathbf{U}) = \mathbf{0}$, that are

$$\begin{aligned} \mathbf{U}_1^* &= (0, 0, 0, 0, 0), & \mathbf{U}_2^* &= (K(b-m), 0, 0, 0, 0), \\ \mathbf{U}_3^* &= \left(\frac{\tau(m+\mu)}{\epsilon\gamma}, \frac{\tau\hat{E}}{\epsilon}, \hat{E}, 0, 0 \right) \quad \text{with } \hat{E} = \frac{1}{\gamma} \left[(b-m) - \frac{\tau(m+\mu)}{\epsilon\gamma K} \right]. \end{aligned} \quad (6.15)$$

The first two equilibria, which represent the trivial and the disease-free states always exist, since we assumed $b > m$. The third equilibrium, that represents the coexistence state, exists if the carrying capacity K satisfies

$$K > K_c = \frac{\tau(m+\mu)}{\epsilon\gamma(b-m)}. \quad (6.16)$$

The subsequent analysis is devoted to give an insight into the behavior of these equilibria with respect to uniform and nonuniform perturbations by assuming K as control parameter. First of all, we linearize system (6.1,6.6) around \mathbf{U}^* for small space and time dependent perturbations of the form

$$\mathbf{U} = \mathbf{U}^* + \hat{\mathbf{U}} e^{\sigma t + ikx}, \quad (6.17)$$

where $\sigma \in \mathbb{C}$ is the growth factor and k is the wave number. Then, inserting (6.17) into (6.1,6.6), we get

$$[\sigma \mathbf{I} - (\nabla_{\mathbf{U}} \mathbf{B})^* + ik \mathbf{A}^*] \hat{\mathbf{U}} = \mathbf{0} \quad (6.18)$$

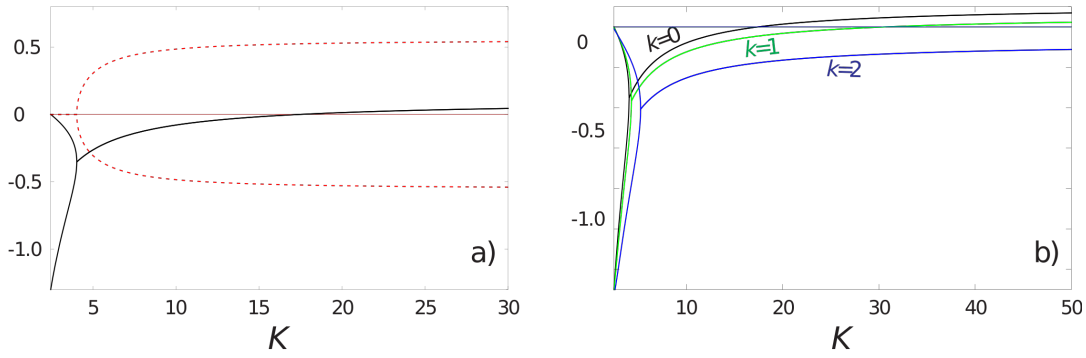


FIGURE 6.1: Fig.1a: Real (black) and imaginary (red) parts of the two complex roots of Eq.(6.24) in terms of the control parameter K . In Figure 1b, such a dependence is illustrated for both homogeneous ($k = 0$) and non-homogeneous perturbations ($k = 1$ and $k = 2$). The graphs are obtained using the values in Table 1, $D_S = 0.1$ and $D_I = 0.01$, $\varphi'(S) = \chi'(I) = 10^3$.

with \mathbf{I} the identity matrix, $\nabla_{\mathbf{U}}$ the gradient with respect to the field variables whereas the asterisk stands for the evaluation of the quantities at \mathbf{U}^* . System (6.18) admits a non-trivial solutions if the following characteristic equation holds

$$\det [\sigma \mathbf{I} - (\nabla_{\mathbf{U}} \mathbf{B})^* + ik \mathbf{A}^*] = 0 \quad \forall \sigma. \quad (6.19)$$

For the trivial state \mathbf{U}_1^* the characteristic equation (6.19) becomes

$$\begin{aligned} & \left[\sigma^2 - \left(b - m + \frac{\varphi'}{D_S} \right) \sigma + \frac{(b-m)\varphi'}{D_S} + k^2 \varphi' \right] \times \\ & \times \left[\sigma^2 + \left(m + \mu + \frac{\chi'}{D_I} \right) \sigma + \frac{(m+\mu)\chi'}{D_I} + k^2 \chi' \right] (\sigma + \tau) = 0, \end{aligned} \quad (6.20)$$

whose solutions can be easily determined. Since at least one solution has positive real part, we can conclude that the empty equilibrium state \mathbf{U}_1^* is unstable.

For the disease-free state \mathbf{U}_2^* the characteristic equation (6.19) becomes

$$\begin{aligned} & \left[\sigma^2 + \left(b - m + \frac{\varphi'}{D_S} \right) \sigma + \frac{(b-m)\varphi'}{D_S} + k^2 \varphi' \right] \times \\ & \times \left\{ \left(\sigma + \frac{\chi'}{D_I} \right) [(\sigma + (m + \mu)) (\sigma + \tau) - K \gamma \epsilon (b - m)] + k^2 \chi' \right\} = 0. \end{aligned} \quad (6.21)$$

It is easy to see that two solutions have negative real parts. In order to understand the signs of the other three real parts, we write explicitly the second factor of (6.21) as

$$\sigma^3 + a_1 \sigma^2 + a_2 \sigma + a_3 = 0 \quad (6.22)$$

with suitable coefficients a_i . Following the Routh-Hurwitz criterium, which asserts that the real parts of these three solutions are negative if

$$a_1 > 0, \quad a_3 > 0, \quad a_1 a_2 > a_3, \quad (6.23)$$

it is easy to ensure that the equilibrium state \mathbf{U}_2^* is stable if $K < K_c$.

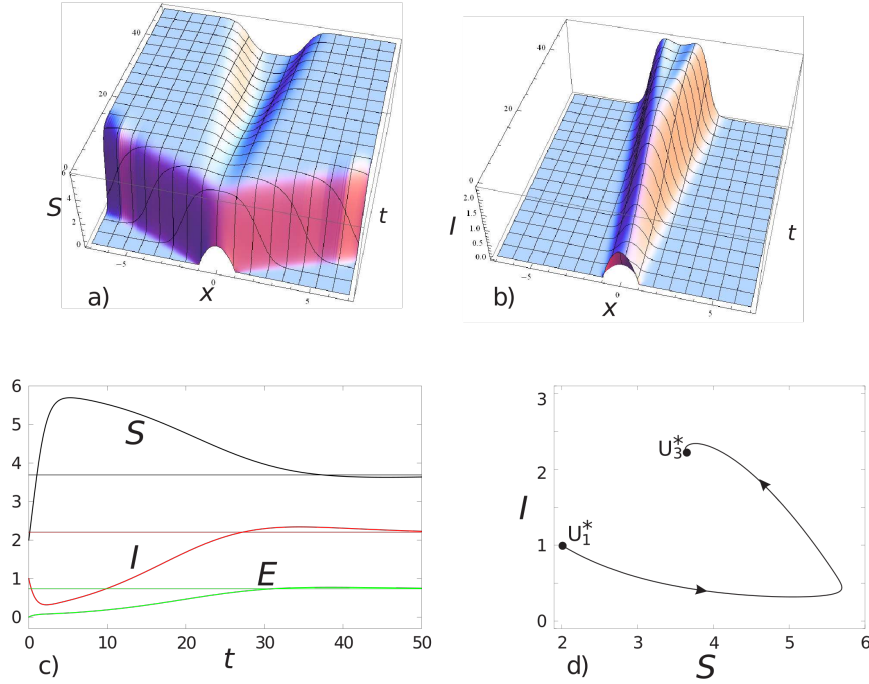


FIGURE 6.2: Solution of the PDE's (6.1,6.6) obtained with the values in Table 1, $D_S = 0.1$, $D_I = 0.01$, $\varphi'(S) = \chi'(I) = 10^3$ and $K = 4$. Fig.2a,b show susceptibles and infected in terms of x and t . In Fig.2c,d the time dependence of the solutions at $x = 0$ is presented with the corresponding trajectory described in the phase plane. The solution illustrates as a little initial perturbation evolves in time and diffuses in space, till the constant equilibrium state U_3^* is reached.

Finally, the characteristic equation (6.19) evaluated in the coexistence state U_3^* becomes a 5th degree polynomial in σ of the form

$$\sigma^5 + \hat{a}_1\sigma^4 + \hat{a}_2\sigma^3 + \hat{a}_3\sigma^2 + \hat{a}_4\sigma + \hat{a}_5 = 0 \quad (6.24)$$

with suitable coefficients \hat{a}_i . Following the Routh-Hurwitz criterium for a 5th order polynomial, the coexistence state U_3^* is stable if

$$\begin{aligned} \hat{a}_1 > 0, \quad \hat{a}_3 > 0, \quad \hat{a}_1\hat{a}_2 > \hat{a}_3, \quad \hat{a}_1\hat{a}_2\hat{a}_3 + \hat{a}_1\hat{a}_5 > \hat{a}_3^2 + \hat{a}_1^2\hat{a}_4, \\ \hat{a}_1\hat{a}_2\hat{a}_3\hat{a}_4 + \hat{a}_2\hat{a}_3\hat{a}_5 + 2\hat{a}_1\hat{a}_4\hat{a}_5 > \hat{a}_3^2\hat{a}_4 + \hat{a}_1^2\hat{a}_4 + \hat{a}_1\hat{a}_2^2\hat{a}_5 + \hat{a}_5^2. \end{aligned} \quad (6.25)$$

Under the assumption of small relaxation times, it is possible to prove that the coexistence state U_3^* is stable if the the carrying capacity K satisfies

$$\begin{aligned} K_c < K < K_H \quad \text{with} \\ K_H &= \frac{\tau(m+\mu) + (m+\mu+\tau)^2 + \sqrt{[\tau(m+\mu) + (m+\mu+\tau)]^2 + 4\tau(b-m)(m+\mu)(m+\mu+\tau)}}{2(b-m)\gamma\epsilon}. \end{aligned} \quad (6.26)$$

For $K > K_H$ the coexistence state U_3^* become unstable and a Hopf bifurcation occurs with a limit cycle surrounding U_3^* .

The results here obtained are in complete agreement with the analogue ones for the parabolic case [Barbera, 2020]. Furthermore, when $k = 0$, they correspond to those of the ODE model in [Sharp and Pastor, 2011], where the space variable is not

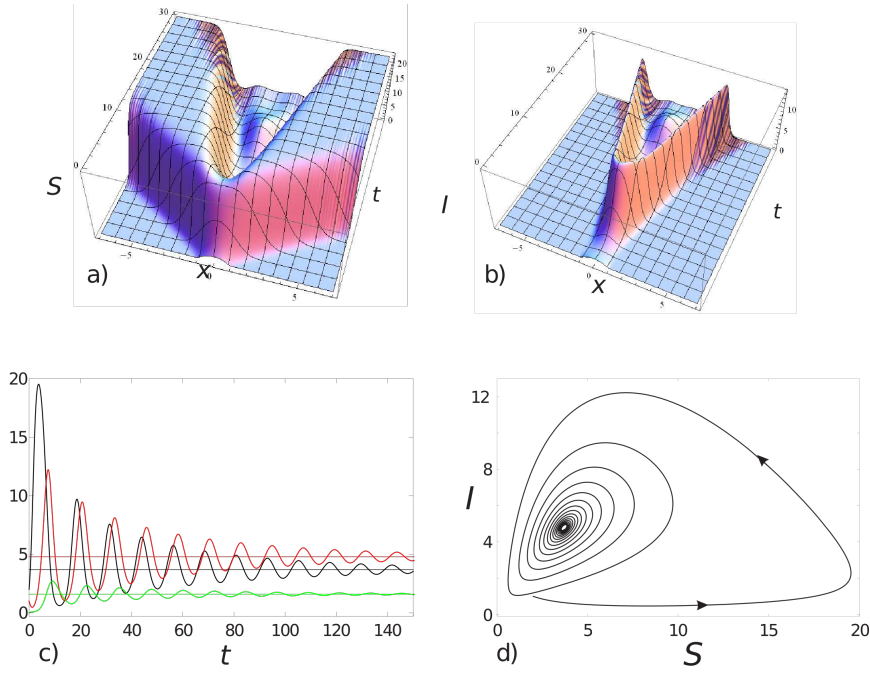


FIGURE 6.3: Solution of the PDE's (6.1,6.6) obtained with the values in Table 1, $D_S = 0.1$, $D_I = 0.01$, $\varphi'(S) = \chi'(I) = 10^3$ and $K = 15$. Fig.3a,b show susceptibles and infected in terms of x and t . In Fig.3cd the time dependence of the solutions at $x = 0$ is presented with the corresponding trajectory described in the phase plane. The solution illustrates as a little initial perturbation evolves in time and diffuses in space till when the constant equilibrium state \mathbf{U}_3^* is reached after some oscillations.

taken into account.

6.4 Numerical investigation

Numerical investigation reveals that equation (6.24) has always three real negative roots, while the other two solutions change depending on K . In Fig.1 both real and imaginary parts of these two roots are plotted versus K . In Fig.1a shows their behavior for $k = 0$, while Fig.1b illustrates their real parts for different k .

From Fig.1a follows that, for $K_c \cong 2.5 < K < 4.3$ the characteristic polynomial (6.24) admits two real negative solutions, therefore the equilibrium \mathbf{U}_3^* is stable. This behavior corresponds to the numerical solution of the field equations (6.1,6.6) shown in Fig.2 that is obtained for $K = 4$, the initial condition

$$S(0, x) = 2I(0, x) = 2 \begin{cases} 1 - x^2 & \text{for } -1 < x < 1 \\ 0 & \text{otherwise} \end{cases} \quad (6.27)$$

vanishing $E(0, x)$ and fluxes.

For $4.3 < K < K_H \cong 17.5$ the two roots of the characteristic polynomial (6.24) are complex with negative real parts (Fig.1). In this case, the constant equilibrium state \mathbf{U}_3^* is stable. Due to the complex parts, the numerical solution of the whole system of field equations (6.1,6.6) tends to \mathbf{U}_3^* with oscillations, as shown in Fig.3 obtained with $K=15$.

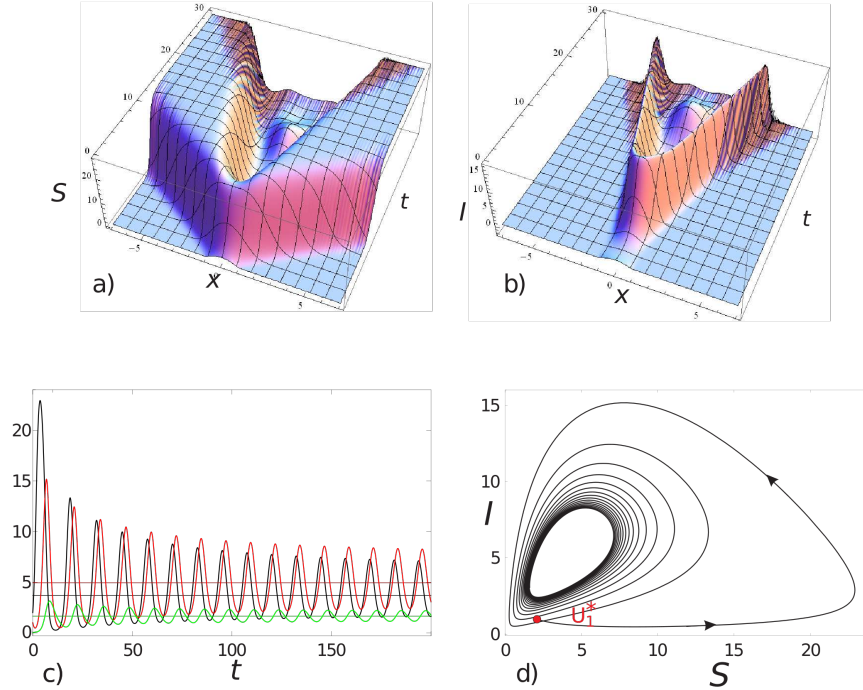


FIGURE 6.4: Solution of the PDE's (6.1,6.6) obtained with the values in Table 1, $D_S = 0.1$, $D_I = 0.01$, $\varphi'(S) = \chi'(I) = 10^3$ and $K = 18$. Fig.4a,b show susceptibles and infected in terms of x and t . In Fig.4cd the time dependence of the solutions at $x = 0$ is presented with the corresponding trajectory described in the phase plane. The figure illustrates as a little initial perturbation evolves in time and diffuses in space till when the stable limit cycle around the unstable state U_3^* is reached.

Finally, for $K > K_H \cong 17.5$ the roots of the characteristic polynomial (6.24) are complex with positive real parts (Fig.1). So the constant equilibrium state U_3^* is unstable and a limit cycle occurs. This can be easily seen in Fig.4 obtained integrating numerically the whole system of field equations (6.1,6.6) with $K=18$.

6.5 Acceleration wave

We consider a moving curve called wave front, across which the fields are continuous whereas their first derivatives may be discontinuous Boillat, 1974. As it is well known, the normal speed of propagation V is equal to the eigenvalue evaluated in the unperturbed field U_r whereas the jump of the normal derivative of the fields Π is proportional to the right eigenvector \mathbf{d} evaluated in U_r , that is

$$V = \lambda(U_r), \quad \Pi = \Pi \mathbf{d}(U_r). \quad (6.28)$$

The amplitude Π of the jump satisfies the Bernoulli equation Boillat, 1974

$$\frac{d\Pi}{dt} + \alpha(t) \Pi^2 + \beta(t) \Pi = 0 \quad (6.29)$$

where $d/dt = \partial/\partial t + \lambda(U_r) \partial/\partial x$ stands for the time derivative along characteristic lines. If the unperturbed state coincides with a constant equilibrium U^* , the

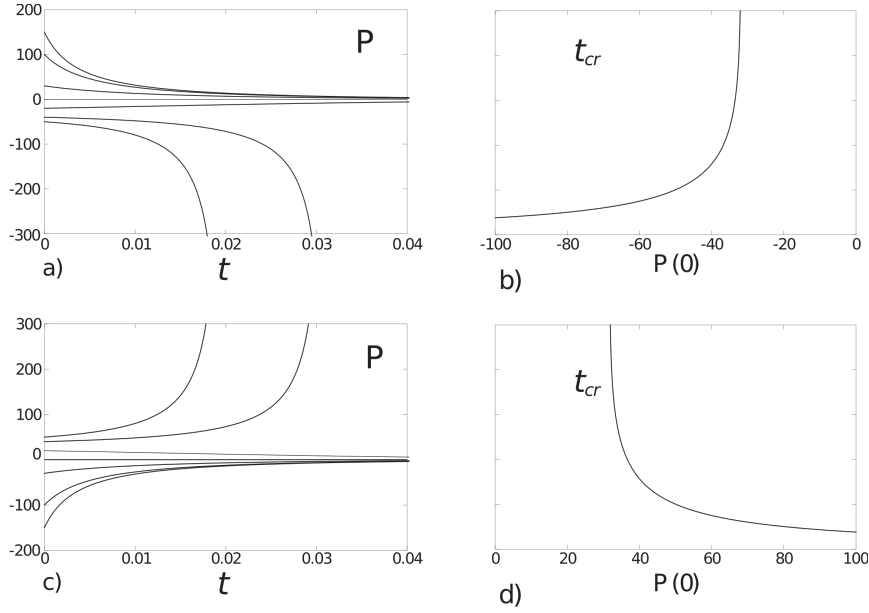


FIGURE 6.5: Acceleration waves and critical time obtained from (6.31,6.32) with the values in Table 1, $D_S = 0.1$, $D_I = 0.01$ Barbera, 2020, $\varphi'(S) = \chi'(I) = 10$ and $\varphi''(S) = 10$ (Fig. 5a,b) or $\varphi''(S) = -10$ (Fig. 5c,d). In Fig5a, since the $\beta < 0$, if $\Pi(0) > -\beta/\alpha \simeq -31$ the initial perturbation $\Pi(0)$ is attenuated and the wave amplitude evolves rapidly to zero. If $\Pi(0) < -\beta/\alpha$ the initial discontinuity is too strong to be attenuated, so it becomes unbounded and the acceleration wave evolves into a shock wave at the critical time illustrated in Fig.5b in terms of the initial amplitude. Fig.4c,d illustrate a different situation, when $\varphi''(S) < 0$. In this case, the acceleration waves evolve to the shock waves for $\Pi(0) > -\beta/\alpha \simeq 31$.

coefficients $\alpha(t)$ and $\beta(t)$ become constant and they are given by

$$\alpha = (\nabla_{\mathbf{U}} \lambda \cdot \mathbf{d})^*, \quad \beta = -(\mathbf{1} \cdot \nabla_{\mathbf{U}} \mathbf{B} \cdot \mathbf{d})^*. \quad (6.30)$$

So integration of the Bernoulli equation leads to

$$\Pi(t) = \frac{\Pi(0) \beta e^{-\beta t}}{\beta - \Pi(0) \alpha (e^{-\beta t} - 1)} \quad (6.31)$$

being $\Pi(0)$ the initial wave amplitude. From equation (6.31) we observe that if $\alpha \neq 0$ the discontinuity becomes unbounded so that the acceleration waves may evolve into shock waves at the critical time

$$t_{cr} = \frac{1}{\beta} \ln \frac{1}{1 - \frac{\Pi_{cr}}{\Pi(0)}} \quad \text{with} \quad \Pi_{cr} = -\frac{\beta}{\alpha}. \quad (6.32)$$

γ	μ	ϵ	m	b	$1/\tau$
0.787 yr ⁻¹	0.567 yr ⁻¹	0.111 yr ⁻¹	0.4 yr ⁻¹	1.9 yr ⁻¹	3 yr

Table 1: The parameters of the model [Miller, Hobbs, and Tavener, 2006].

In order to show the behavior of acceleration waves, we evaluate α and β in the more interesting equilibrium state \mathbf{U}_3^* . The obtained values are

$$\begin{aligned}\alpha_{1,2} &= \pm \frac{\varphi''(S_3^*)}{2\sqrt{\varphi'(S_3^*)}} & \alpha_{3,4} &= \pm \frac{\chi''(I_3^*)}{2\sqrt{\chi'(I_3^*)}} \\ \beta_{1,2} &= \frac{(m+\mu)\tau}{2K\gamma\epsilon} + \frac{\varphi'(S_3^*)}{2D_S} > 0 & \beta_{3,4} &= \frac{m+\mu}{2} + \frac{\chi'(I_3^*)}{2D_I} > 0\end{aligned}\quad (6.33)$$

Figure 5 shows the results for the acceleration waves propagating with velocity $V = \lambda_1 = \sqrt{\varphi'(S)}$ in the constant state \mathbf{U}_3^* assuming the derivative $\varphi''(S_3^*)$ a positive or a negative function. In Fig.5_{a,c} the behavior of the dimensionless amplitude $\Pi(t)$ for different values of $\Pi(0)$ is shown, while in Fig.5_{b,d} the critical time is depicted (where it exists) as a function of the initial amplitude.

6.6 Conclusion and final remarks

In this Chapter an hyperbolic model is introduced in the context of Extended Thermodynamics which generalizes the ODE model in [Sharp and Pastor, 2011] and the parabolic one [Barbera, 2020]. By analytical calculations and numerical solutions was shown that, when the relaxation times are small, the hyperbolic model has the same characteristic of the parabolic one [Barbera, 2020]. For higher values of the relaxation times, the study of the acceleration waves is illustrated and the evolution of initial perturbation in the derivatives is depicted together with the critical time. The model can be generalized to the two dimensional case, providing more general results.

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