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Project Report

Simulations of electron concentration in the wake of meteors and application to radio observations

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Abstract

The entry of meteoroids in the Earth's atmosphere is characterized by high velocities, reaching 72 km/s. At such velocities, extremely high temperatures are reached and the meteoroid is surrounded by a region of plasma, dense enough to be detected by ground-based radio stations. The Belgian RAdio Meteor Stations (BRAMS) network is a unique experiment based on 30 receivers spread all over Belgium to collect and standardize meteor observations. Correlating the physical parameters of the incoming meteoroid to the reflected radio signal requires a simulation of the plasma flow that develops around the hypersonic body and into its trail.

Detailed chemistry models are usually too computationally expensive to be strongly coupled to flow solvers. This project aims at simulating the ionized trail past a meteoroid by coupling standard flow solvers to a lightweight Lagrangian solver developed at VKI, allowing to introduce *a posteriori* an arbitrarily complex chemistry into the model.

The first and main part of this work deals with the extension of the existing VKI Lagrangian solver capabilities, to include mass and energy diffusion mechanisms. The developed code is verified against simple testcases. Simulations of meteors at high altitute are then performed using the Direct Simulation Monte Carlo (DSMC) method, and a knowledge of the fluid dynamics behavior of the trail is built. Since those simulations are deficient from the chemical point of view, the Lagrangian solver is applied in order to introduce a detailed chemistry, including in particular recombination reactions for free electrons. This provides a much more reliable estimation of the free electrons density in the meteor trail with respect to the initial DSMC simulations. Finally, the Lagrangian solver is applied to the study of very long trails, providing a map of free electrons up to a distance of 2 km from the meteoroid. The tool and methodology developed in this work allow to study the properties of meteor trails in a computationally efficient way, up to very big lengths. Maps of free electrons obtained in this work can be correlated to experimental signals of the BRAMS network by use of an electromagnetic solver.

A number of different fields may benefit from the developed code. Possible applications include the study of blackout phenomena occurring during the reentry of spacecrafts, determination of the electrons recombination and energy levels population in the plume of ion thrusters, characterization of armospheric entry of space debris and may even be applied to the radio detection of ICBM missiles.

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List of Symbols

Acronyms

LTE	Local Thermodynamic Equilibrium
RRHO	Rigid Rotor-Harmonic Oscillator
HS	Hard Sphere
VHS	Variable Hard Sphere
VSS	Variable Soft Sphere
TCE	Total Collision Energy
VKI	von Karman Institute

Roman symbols

Kn	Knudsen number	
Da_III	third Damköhler parameter	
$f^{\mathcal{M}}$	Maxwellian distribution	s^3/m^6
k_B	Boltzmann constant	J/kg/K
\mathcal{D}_{ert}	diffusion matrix	m^2/s
Y_i	mass fraction	
X_i	mole fraction	
V_i^d	diffusion velocity	m/s

Greek symbols

- streamline slope α
- β ionization coefficient
- λ mean free path m
- collision deflection angle ξ rad m^2
- collision cross section σ
- kg/schemical production term $\dot{\omega}$

Chapter 1

Introduction

«I've seen it rainin' fire in the sky» John Denver Rocky Mountain High

Every year, around the 10th of August, the summer night sky fills with meteors. Catholic culture depicts them as the tears of saint Lawrence, burned alive during the Roman empire. Others say shooting stars are the souls of new babies, traveling towards the sky to reach the Earth.



Figure 1.1: Visualization of a meteor.

Falling stars recently became a research interest of the von Karman Institute for Fluid Dynamics, not for their astonishing beauty, but because of the scientific knowledge they carry with them. In fact, *meteors* originate from the atmospheric entry at very high velocities of debris originating from comets or asteroids, referred to as *meteoroids*. Developing methods for studying meteors allows to discover precious information over the composition and the characteristics of their parent bodies, without need for space expeditions.

The quantity of such meteoroids daily entering the Earth's atmosphere amounts to around 50 tons, of which the vast majority is totally destroyed even before they can reach the ground, due to their very small size (μ m to m in diameter) and extremely high flight velocity (up to 72 km/s).

The study and characterization of the meteoric phenomenon is of big importance not only for astronomy, but for aerospace engineering as well, since the physical phenomena experienced by meteoroids during their atmospheric entry are the same that characterize the reentry of aerospace vehicles and space debris such as satellites at their end of life. Meteors provide flight data at zero cost, for conditions that are even more severe than those encountered by spacecrafts (whose typical speed ranges from 5 to 14 km/s): this allows us to extend the validity range of currently employed methods.

1.1 Radio observation of meteor trails

As anticipated, the meteor phenomena is generated by the atmospheric entry at very high velocity of bodies coming from space, whose origin is well explained by Murad and Williams in [1] and by Ceplecha et al. in [2]. During the atmospheric entry, the air flow is strongly heated and the temperature reaches values in the order of 100 000 K. At such temperatures, the collisions among air molecules are so strong that chemical reactions take place. In particular, ionizing reactions produce a number of free electrons, that are released in the meteor trail.

Chemical reactions among air species are not the only source of free electrons, in fact at the extremely high temperatures met by the meteoroid, its surface starts melting and vaporizing and a quantity of ablated species mix with the fluid flow, starting reacting as well. This effect is known to produce a significant number of electrons since the ionization energy of species that compose the meteoroid is *much lower* than that of air species. Fig. 1.2 sketches the main phenomena involved in this atmospheric entry phase.



Figure 1.2: Sketch of phenomena experienced by a meteoroid during its entry.

One of the techniques used to detect meteors consists in exploiting the scattering process that radio waves experience when they cross ionized regions of space (Fig. 1.4). In this technique, a transmitter antenna radiates a signal in the MHz range and when a meteor passes in the surrounding area, the signal is reflected by the electrons in the trail and can be gathered by a network of receiver antennas, as reviewed by Wislez in [3].

The Belgian Institute for Space Aeronomy is currently taking part in the study of meteors via radio observations, with the BRAMS project [4], a unique network of 30 ground-based stations, aiming at collecting and standardize meteor observations. A large number of meteoric echoes is collected each day (in average, one observation per minute over Belgium), and by crossing the data from various receivers it is possible to reconstruct the trajectory of the falling body [5].



Figure 1.3: Scheme of the radio forward scattering technique for meteor detection.



Figure 1.4: Example of signal from a BRAMS network station.

While the velocity and trajectory of the meteoroid can be directly reconstructed from the received signal, inferring characteristics such as the meteoroid's mass and size additionally requires an accurate modeling of the electron density in the trail. This process is composed by two steps:

- i) the amount of free electrons in the trail needs to be accurately described as a function of the meteoroid size, velocity and composition, as well as altitude;
- ii) the scattering of the radio wave in the ionized region has to be computed.

Current research in this field relies on strong approximations. First of all, the flowfield is not modeled: a global effect of the interaction between ablated species and air constituents is given by the ionization coefficient β [6], following a 0-D approach. The number density of free electrons n_e is then computed as a function of flight velocity V_{∞} , ablation rate \dot{m} and ionization coefficient: $n_e = f(V_{\infty}, \dot{m}, \beta)$, as shown by Baggaley in [7]. This project deals with providing a more sound modeling of the electrons number density, by providing a complete fluid dynamic description.

A second strong simplification is employed in the current literature regarding the interaction of the radio wave with the meteor trail. Given the electron density and the corresponding parameter *plasma frequency*, see Bellan [8], the trail is divided in two regions where different scattering mechanisms apply: the *underdense* and *overdense* trail types. Different simplifications are introduced for the two families, namely assuming a given cross-sectional profile for the electrons number density (for underdense meteors) or a total reflection of the incoming radio wave in case of overdense meteors, see [9, 10, 11]. Those models lead to a qualitative explanation of the shape of the reflected signal, and could be improved by numerical simulations once the concentration of free electrons is accurately known.

Regarding the description of the free electrons, the ablation of meteoroid constituents plays a central role: using spectroscopic measurements [12] and analyzing meteorites retrieved on the ground, the composition is found to be rich in metals such as Fe, Mg and Na, whose ionization energy is *much lower* than that of air species. Chemical reactions involving those elements are thus to be taken into account if an accurate description of free electrons is sought [13, 14]. Despite the importance of ablation, its effects will not be considered in this project: the tools developed will be flexible enough to consider ablated species, once more details and accurate chemical rates will be available.

1.2 Numerical simulation of reactive rarefied flows

Numerical efforts are well under way at VKI for modeling the interaction of meteors with the atmosphere, see Bariselli [15] and Dias [16]. Those efforts are focused respectively in the rarefied and continuum regime. In fact, during its atmospheric entry, a meteor crosses two different fluid dynamics regimes. The first part of the trajectory is characterized by a large Knudsen number, ratio of the mean free path for the gas molecules and a characteristic length (such as the meteor diameter), the atmosphere is rarefied and the flowfield can not be obtained using the Navier-Stokes equations [17]. Thus, approaches based on the solution of the Boltzmann equation are required, the most common example being the Direct Simulation Monte Carlo (DSMC) method introduced by Bird [18]. Another approach useful in this regime is the Particle In Cell (PIC) method, applied to meteors by Dyrud et al. [19], specifically designed for taking into account electromagnetic fields in the flow, but neglecting the effect of collisions among particles. At lower altitudes the Knudsen number decreases due to higher atmospheric densities, allowing standard hypersonic CFD simulations to be employed. The challenge of computing the free electrons concentration in the meteor's trail is twofold:

- Detailed chemical mechanisms are required, greatly increasing the computational cost of numerical simulations;
- Simulations are to be performed in two different regimes, where different governing equations apply.

Unfortunately, those challenges prove to be overwhelming for standard fluid dynamics methods. In fact, while they provide reliable tools for studying the flowfield *around* the meteoroid, DSMC and CFD suffer from different limitations when applied to the study of meteoroid trails.

DSMC methods typically suffer from an algorithmic limitation that makes them unable to compute recombination reactions. Free electrons produced by energic collisions diffuse in the surroundings but never recombine with positive ions. While this is not an issue for the the study of ionized flows *around* hypersonic bodies, this is a problem in elongated recombining trails, in that a DSMC simulation would predict a number of electrons which is constant over each trail cross section, at whatever distance, which is not the case in reality.

On the other hand, CFD methods become extremely heavy when a big number of reactions is to be taken into account. In fact, for each chemical species introduced, one mass equation has to be added to the system to be solved. Since the number of species is *very* high (air brings 11 species to the balance and if ablation is to be modeled the number of species increases quickly) the system becomes prohibitively large.

Moreover, the domain size is extremely extended (of the order of 1 km), posing additional troubles to classical numerical simulations. The answer to the exposed problems will be detailed in the next section.

1.3 Aim and structure of this work

This work aims at providing a numerical methodology for studying the free electrons concentration in meteor trails. The procedure that will be formulated aims at being sound from the fluid dynamics point of view, which constitutes a big improvement over the current state of the art.

The answer of this work to the numerical difficulties encountered by classical fluid dynamics solvers will lie in the development of a particular Lagrangian solver, whose lightweight structure will allow to easily introduce detailed chemical models.

The aim of this work is thus twofold:

- 1. Development of a Lagrangian flow solver for detailed chemistry, plus its verification;
- 2. Development of a methodology for modeling the electron concentration field in meteor trails, together with the analysis of a chosen testcase.

First of all the governing equations describing chemically reacting and rarefied flows will be introduced in Chapter 2, together with the physico-chemical models for high enthalpy flows (Chapter 3). Attention will then switch to numerical methods: in Chapter 4, the Direct Simulation Monte Carlo method will be introduced, while Chapter 5, deals with the main numerical contribution of this work: the creation of a Lagrangian solver able to treat detailed chemical models. Finally, in Chapter 6 a methodology for analyzing meteor trails is suggested and applied to a meteor testcase, leading to a map of free electrons up to 1 km of distance from the meteoroid.

Chapter 2

Governing equations

The year 1822 is particularly important to fluid dynamicists. One could state that the modern fluid dynamics was born in this year, when a famous contribution was presented to the French Académie royale des Sciences. This contribution is the celebrated "Mémoire sur les lois du mouvement des fluides" by Claude-Louis Navier, where for the first time a realistic mathematical description for viscous flows is presented.

This contribution constitutes a giant leap with respect to the previous inviscid modeling of fluid flows, so big that most engineers and scientists have the feeling that fluid dynamics is now complete. Since the settling of the Navier-stokes equations, many believe that "this is the whole story". However, this is not the case.

Half a century passes, and the next big step knocks on the door of fluid dynamics: this time it's Ludwig Boltzmann, whose equation brings the flow modeling to the next level. In fact, the Navier-Stokes equations suffer from a serious disadvantage: they lose their validity when the flow is highly out of equilibrium. High Knudsen number flows such as rarefied gases or flows inside small-scale devices are probably the most famous cases where this breakdown arises.

Many more derivations were proposed in the following years and important milestones were set, one of them being the Vlasov equation for plasma flows for example.

This chapter is dedicated to the mathematical models that will be used in this work for describing the ionized flow developing in rarefied meteor trails. While the abundant presence of free electrons in meteor trails suggests the Vlasov equation as most logical framework, the characteristics of meteor flows are such that they can be classified as *unmagnetized plasmas*. As such, the main issue to be taken into account for modeling high altitude meteoric flows is non-equilibrium and consequently this chapter will focus on the Boltzmann equation, together with their fluid-flow counterpart: the Maxwell transfer equations, generalization of the Navier-Stokes equations.

2.1 From microscopic to macroscopic description

As is well known, the physical nature of fluids is non continuum: fluids are composed by a finite number of atoms and molecules, exchanging energy and momentum through collisions. A description of the physics at this *microscopic scale* needs to take into account intermolecular potentials and mechanisms of internal excitation of molecules and atoms. However, fluids have been described since centuries starting from global conservation equations (such as the Navier-Stokes equations): description was thus performed at a *macroscopic scale*, and it proved to be successful in most circumstances.

It is now clear that the behavior of a fluid at the macroscopic scale depends on the collective behavior of the particles that constitute it. Probably, the beauty of the modern fluid dynamics theory lies in the fact that a link between those two microscopic and macroscopic words is now established (even though a rigorous mathematical proof is still missing). This link is settled in the elegant framework of kinetic theory.

In fact, the microscopic world is the starting point of the Boltzmann equation, that describes how a population of particles evolves in time, from the statistical point of view. From this information, it is possible to obtain all the fluid dynamic information that fluid dynamicists use in their daily practice: velocity field, temperature, density and so on.

Of course, dealing with global conservation equations is easier than approaching the Boltzmann equation, let's thus start by the reason that leads engineers towards the microscopic approach as the degree of rarefaction of a flow increases.

Knudsen number and breakdown of Navier-Stokes equations

An indication of the degree of rarefaction of a fluid flow is provided by the Knudsen number Kn, defined as the ratio of molecular mean free path λ and characteristic dimension L of the flow:¹

$$Kn = \frac{\lambda}{L}$$
(2.1)

Flows characterized by Knudsen numbers much smaller than unity are said to be in the *continuum regime* and the Navier-Stokes equations usually hold. The threshold is typically set to the value $\text{Kn} \approx 0.01$. On the other extreme, Knudsen numbers larger than $\text{Kn} \approx 10$ characterize the so called *molecular regime*, where collisions among molecules are unlikely to happen due to the very large mean free path. In the middle, flows partially deviate from the Navier-Stokes prediction: from $\text{Kn} \approx 0.01$ to 0.1 there is the *slip regime*, while the range from $\text{Kn} \approx 0.1$ to 10 is named *transition regime*.

Of course, such description is quite coarse and the continuum model may break *locally*: it is possible to define the Knudsen number via the *local* gradients of a flow property Q:

$$\operatorname{Kn} = \frac{\lambda}{Q} \left| \frac{\mathrm{d}Q}{\mathrm{d}x} \right| \tag{2.2}$$

In the current work, a meteoroid with a diameter of 1 cm will be simulated at the altitude of 70 km. At such conditions, the Knudsen number is found to be approximately Kn = 0.1 and the flow is thus located at the border between the slip and the transition regimes. For this reason, a description based on the continuum should not be trusted, and a microscopic approach is required.

 $^{^{1}}$ In case of a space vehicle entering the rarefied layers of the atmosphere, this dimension may be taken as the vehicle diameter.

A bridge from microscopic to macroscopic world

The statistical treatment of fluid flows from the microscopic point of view is based on the definition of the velocity distribution function $f(\boldsymbol{x}, \boldsymbol{c}, t)$, describing the probability that a particle with velocity between \boldsymbol{c} and $\boldsymbol{c} + d\boldsymbol{c}$ is located at a position between \boldsymbol{x} and $\boldsymbol{x} + d\boldsymbol{x}$ at the time t.

Macroscopic flow quantities are readily obtained by integrating over the velocity space. The value of the flow density, momentum and energy for a pure gas would read:

$$\begin{cases} \rho(\boldsymbol{x},t) = \int m f(\boldsymbol{x},\boldsymbol{c},t) \, \mathrm{d}\boldsymbol{c} \\ \rho \boldsymbol{u}(\boldsymbol{x},t) = \int m \, \boldsymbol{c} \, f(\boldsymbol{x},\boldsymbol{c},t) \, \mathrm{d}\boldsymbol{c} \\ E(\boldsymbol{x},t) = \int \frac{1}{2} \, m \, |\boldsymbol{c}|^2 f(\boldsymbol{x},\boldsymbol{c},t) \, \mathrm{d}\boldsymbol{c} \end{cases}$$
(2.3)

where m is the mass of the particles and the integral is performed over the three components of the velocity c. For the case of a multispecies gas such as air, the same result is obtained by summing over the species:

$$\begin{cases} \rho(\boldsymbol{x},t) = \sum_{i} \int m_{i} f_{i}(\boldsymbol{x},\boldsymbol{c}_{i},t) \,\mathrm{d}\boldsymbol{c}_{i} \\ \rho \boldsymbol{u}(\boldsymbol{x},t) = \sum_{i} \int m_{i} \,\boldsymbol{c}_{i} f_{i}(\boldsymbol{x},\boldsymbol{c}_{i},t) \,\mathrm{d}\boldsymbol{c}_{i} \\ E(\boldsymbol{x},t) = \sum_{i} \int \frac{1}{2} m_{i} \,|\boldsymbol{c}_{i}|^{2} f_{i}(\boldsymbol{x},\boldsymbol{c}_{i},t) \,\mathrm{d}\boldsymbol{c}_{i} \end{cases}$$
(2.4)

The expression for other macroscopic quantities can be found multiplying the distribution function by different terms, see Giovangigli [20]. This multiplication process can be seen as a weighting of the distribution function, and the integral of the obtained quantity is referred to as a moment of the distribution function. The energy for example is found as an average of the particles kinetic energy $\frac{1}{2}m_i |\mathbf{c}_i|^2$.

This theory thus provides the link between the microscopic and the macroscopic worlds. The same treatment can be employed to obtain global conservation equations starting from microscopic equations such as the Boltzmann equation, as will be discussed in the next chapters.

2.2 The Boltzmann equation

The celebrated (and feared by most engineers) Boltzmann equation describes the evolution in time of the distribution function $f_i(\boldsymbol{x}, \boldsymbol{c}_i, t)$. For a multispecies gas mixture, the Boltzmann equation reads:

$$\frac{\partial f_i}{\partial t} + \boldsymbol{c}_i \cdot \boldsymbol{\nabla}_x f_i + \frac{\boldsymbol{F}_i}{m_i} \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_i} f_i = J_i \quad \text{with} \quad i \in \mathcal{S}$$
(2.5)

where \mathbf{F}_i is the external force acting on the particle, such as gravity or Lorentz force in case of charged particles. From an intuitive point of view, its meaning is clear: the time evolution of the distribution function at a given position (the first term) is regulated by an advection term (the second term) and by a term linked to the work of external forces \mathbf{F}_i (third term) and finally by one more term J_i taking into account the effect of collisions among particles. The problem is that the term J_i , named collision integral, has an integral nature and the Boltzmann equation thus becomes an *integro-differential* equation:

$$\begin{cases} J_i = \sum_{j \in S} J_{ij}(f_i, f_j) \\ J_{ij}(f_i, f_j) = \int \left(f'_i f'_j - f_i f_j \right) |\mathbf{c}_i - \mathbf{c}_j| \,\sigma_{ij} \mathrm{d}\omega \mathrm{d}\mathbf{c}_j \end{cases}$$
(2.6)

the meaning of the terms being explained by Cercignani for example in [21]. Its integro-differential nature makes the Boltzmann equation very hard to approach and its *direct* solution can be nowadays obtained only for simple cases.

However, due to its capability of describing both continuum and rarefied flows, the Boltzmann equation results very appealing and indirect numerical strategies for its solution have been developed, such as the Direct Simulation Monte Carlo method.

2.3 Maxwell transfer equations

Just as macroscopic flow properties can be obtained by computing moments of the distribution function, conservation equations can be obtained by computing moments of the Boltzmann equation. The resulting set of equations is often called the *Maxwell transfer* equations and is a set of PDEs expressing the mass, momentum and energy conservation. Being obtained from kinetic theory, those equations are valid both in and out of thermodynamic equilibrium.

$$\partial_t \rho_i + \partial_{\boldsymbol{x}} \cdot (\rho_i \boldsymbol{u}) + \partial_{\boldsymbol{x}} \cdot (\rho_i \boldsymbol{V}_i^d) = \dot{\omega}_i$$

$$\partial_t (\rho \boldsymbol{u}) + \partial_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \partial_{\boldsymbol{x}} \cdot \boldsymbol{\Pi} = nq\boldsymbol{E} + \boldsymbol{j} \times \boldsymbol{B}$$

$$\partial_t (\rho e) + \partial_{\boldsymbol{x}} \cdot (\rho e \boldsymbol{u}) + \partial_{\boldsymbol{x}} \cdot \boldsymbol{q} + \boldsymbol{\Pi} : \partial_{\boldsymbol{x}} \boldsymbol{u} = \boldsymbol{j} \cdot (\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B})$$
(2.7)

where the terms at the right hand side include the effect of the electric field \boldsymbol{E} and magnetic field \boldsymbol{B} on charged particles. The terms appearing are well established in fluid dynamics, except possibly for the term $\dot{\omega}_i$, expressing the rate of production of the *i*-th species due to chemical reactions and the term V_i^d , diffusion velocity of the *i*-th species.

As said, such equations are valid both in and out of thermodynamic equilibrium, meaning that their operational range is extended to the rarefied region. The problem encountered in solving this equations lies in finding a closure for the transport terms: the divergence of the stress tensor Π , the heat flux q and the diffusion velocity V_i^d . The Navier-Stokes equations are just *one* closure possibility, with the advantage of simplicity but carrying the drawback of breaking down as the flow becomes rarefied.

From the kinetic point of view, the Navier-Stokes equations are valid for *small* departures from equilibrium, where the distribution function is closely Maxwellian:

$$f_i^{\mathcal{M}} = n_i \left(\frac{m_i}{2\pi k_B T}\right) \exp\left(-\frac{m_i \left(\boldsymbol{c}_i - \boldsymbol{u}\right)^2}{2k_B T}\right) \quad \text{with} \quad i \in \mathcal{S}$$
(2.8)

where n_i is the number density and k_B the Boltzmann constant. Luckily, despite the high degree of rarefaction, this will prove to be the case in the meteor trails of this work.

Chapter 3

Physico-chemical models for hypersonic flows

If one was to summarize hypersonic flows in just one world, this would probably be "temperature". In fact, at high flight speeds the huge kinetic energy of the flow converts into thermal energy near the body and the temperature raises up to values in the order of 10 000 K for the Apollo capsule entry, and up to 1 000 000 K for meteors. Temperature changes often happen extremely quickly and this is the case of shockwaves for example or hypersonic boundary layer flows.

The description of hypersonic flows fundamentally deviates from classical supersonic aerodynamics for the progressive importance that real gas effects acquire as the flight speed increases. The molecular nature of the flow has to be taken into account and its thermodynamic and transport properties need to be accurately modeled, as well as chemical reactions.

This chapter introduces the main physico-chemical models used in this work for describing the properties of meteor trails.

3.1 Thermodynamic properties

Thermodynamic properties of high temperatures flows are usually obtained from a microscopic approach, where the energy states of atoms and molecules are directly modeled using quantum mechanics.

The energy of elementary particles is distributed among various forms: first of all, atoms and molecules possess *translational energy* due to their motion in space; molecular species also possess *rotational* energy, depending on their geometrical shape and thus to their moment of inertia, and *vibrational* energy due to the intermolecular potential keeping together its constituting atoms. Finally, atoms and molecules both have the ability to store energy in the form of *electronic* energy, originating from the Coulomb interaction between the positively charged nucleus and the bond electrons. An additional contribution is given by the *formation energy*, to be taken into account whenever chemical reactions take place. The case of free electrons is simpler, since they only have translational and formation energies (and their spin).

From all the said types of energy a temperature can be defined, so that for a given chemical species i, the energy per unit mass may be written as:

$$\begin{aligned} i \in \mathcal{M} &\to e_i &= e_i^{tr}(T) + e_i^{rot}(T^r) + e_i^{vib}(T^v) + e_i^{el}(T^e) + e_i^{form} \\ i \in \mathcal{A} &\to e_i &= e_i^{tr}(T) + e_i^{el}(T^e) + e_i^{form} \\ \text{free electrons} &\to e_e &= e_e^{tr}(T_e) + e_e^{form} \end{aligned}$$

where \mathcal{M} and \mathcal{A} refer to the set of molecules and atoms and the appearing temperatures are respectively the translational (T), rotational (T^r) , vibrational (T^v) and electronic (T^e) temperatures¹. The last three are referred to as *internal temperatures*.

Of course, different chemical species may have different internal energies, but this case is out of the scope of this work. In particular, this work will be performed in the somehow simplified hypothesis that all those temperatures are equal: $T = T^r = T^v = T^e$. Such case is referred to as *thermal equilibrium* and appears when a sufficient time interval is left to the chemical species for equilibrating (thermalizing) their energy levels.

The physical expression of those energies, as well as all the thermodynamic properties arising from them (such as specific heats) is obtained in the framework of quantum and statistical mechanics and is very nicely explained in [22].

As a final note, the model used in this work for the molecular energy levels is the *Rigid Rotor Harmonic Oscillator* model (RRHO). The reader is referred to the given reference for additional details.

3.2 Transport properties

While thermodynamic properties can be obtained from quantum and statistical mechanics, an expression for transport properties is typically obtained in the framework of kinetic theory. In fact, transport properties express how mass, momentum and energy are transported among nearby fluid elements and are fundamentally due to the collisions between molecules composing the fluid.

In this work on meteor trails, we are particularly interested in two transport properties: mass diffusion coefficients and heat conductivity. The first property will be used to model the diffusion of free electrons from the core of a ionized meteor trail to the surrounding regions, while the latter will enable us to model how a hot trail cools down and reaches the freestream temperature. Interestingly enough the viscosity, probably the most famous among the transport properties will not be used in this work, due to the particular Lagrangian nature of the tools developed.

A microscopic description of transport properties starts from the modeling of molecular collisions. Molecular collisions can be treated classically as the motion of two bodies with a given initial velocity and an intermolecular potential $\varphi(r)$ among them. From the

¹Note that the assumption that the translational energy of free electrons is equal to the electronic energy of heavy species has been here performed. This is frequently the case since electron collisions are the preferred way of exciting electronic levels of atoms and molecules

potential, the main *collision integrals* $Q_{ij}^{(l,s)}$ can be computed, as reported in [23]. Those quantities then enable transport properties to be computed via algorithms proper of the kinetic theory of gases, as deeply explained in [20].

Mass fluxes

The computation of mass fluxes proceeds through the computation of the diffusion velocities V_i^d , through the diffusion matrix \mathcal{D}_{ij} . Only the gradients of species concentrations will be used as a driving force, while barotropic diffusion and Soret effect will be neglected:

$$\boldsymbol{V}_{i}^{d} = -\sum_{j} \mathcal{D}_{ij} \boldsymbol{\nabla} X_{j} + k_{i} \boldsymbol{E}$$
(3.1)

This is just *one* possibility of obtaining the diffusion velocity, another one being solving the Stefan-Boltzmann equation [20].

Heat flux

The heat flux q will be computed through the thermal conductivity k and taking into account energy trasport through diffusive mass flux:

$$\boldsymbol{q} = -k\boldsymbol{\nabla}T + \sum_{i} \rho_{i}h_{i}\boldsymbol{V}_{i}^{d}$$
(3.2)

Ambipolar assumption

A particularity of low density plasmas, such as meteor plasmas, is the tendency to remain quasi-neutral. In fact, although free electrons detach from heavy species, when external electromagnetic fields are not applied the Coulomb attraction to the positive ions is such that the plasma remains *globally* neutral. Local charge oscillations happen but their extent is limited to the Debye length.

This behavior is the so called *ambipolar assumption*: an ambipolar electric field is created when electrons and ions distantiate from each other, pulling them back together. This behavior has an impact in the way the transport properties are obtained, as reviewed by [20]. Mathematically, this property translates into imposing zero current and charge:

3.3 Chemical reactions

Chemical reactions are a characterizing phenomena of high hypersonic flows. In the framework of meteor trails in particular, attention is focused to ionization and recombination reactions, regulating the quantity of free electrons populating the trail.

Chemical reactions appear in the governing equations trough the term $\dot{\omega}_i$ (eq. 2.7), expressed through the *law of mass action* as explained by Anderson in [24]. In the current work, the chemical rate coefficients k are based on the generalized Arrhenius law:

$$k = AT^n \exp\left(-E_a/k_B T\right) \tag{3.3}$$

where T is the temperature, k_B the Boltzmann constant and E_a the activation energy of the reaction. The parameters A and n, as well as the activation energy are typically obtained by fitting this expression to experimental data. This form is almost ubiquitously used in hypersonic gas flows and the chemical mechanism for air, as well as the rates constants A, n and E_a , are taken from Park [25].

3.4 The Mutation++ library

From a practical point of view, the thermodynamic and transport properties needed in this work are obtained via the Mutation++ library (MUlticomponent Thermodynamic And Transport properties for IONized gases in C++). Such a library is an open-source tool developed at VKI, aimed at providing an efficient coupling with CFD codes.

Enthalpies, specific heats, chemical rates and diffusion coefficients at a given thermal state are easily obtained by a call to the library, and can be plugged into the governing equations describing the flow behavior.

As an example of the capabilities of the Mutation++ library, a plot of the enthalpy and specific heat at constant pressure is shown in Fig. 3.1. The gas is an air mixture composed by 11 species: N_2 , O_2 , N, O, NO, N_2^+ , O_2^+ , N^+ , O^+ , NO^+ and free electrons e^- . The enthalpy and specific heat are plotted at various temperatures characteristic of the hypersonic regime, and shows the classical behavior of reacting flows: in fact, peaks are obtained in correspondence of the dissociation of chemical species, where part of the energy is used to break molecular bonds or, at higher temperatures, to ionize the flow.

The Mutation++ library is used in all the simulations performed by the Lagrangian reactor LARSEN developed in this work. This library is used also in Appendix C.



Figure 3.1: Mutation++: enthalpy and specific heat at various temperatures for the air 11 mixture at 100 Pa.

Chapter 4

DSMC method for rarefied flows

In Chapter 2 the equation describing the behavior of flows up to high degrees of rarefaction was introduced: the Boltzmann equation. As was explained, a direct solution of such equation is hard to obtain due to its integro-differential nature. This section deals with the most used indirect approach for obtaining a solution the Boltzmann equation: the Direct Simulation Monte Carlo (DSMC) method, first introduced by G. Bird and well treated in [18].

4.1 DSMC algorithm

The DSMC method mimics the physical nature of gases, that are composed by a large number of particles, exchanging energy with each other via molecular collisions. The method treats the motion of particles deterministically but relegates collisions to the statistics. In particular, the method is composed by two steps:

Translation step: particles are moved in the domain following a ballistic trajectory

Collision step: collisions are computed among randomly sampled pairs of particles.

It's important to recall at this step that DSMC is not molecular dynamics, in that only a very small subset of particles is actually simulated. Those simulated particles have the very same physical properties as real particles, but are representative of a large number of them. The correct solution is then obtained through the statistical treatment of the results. This fact allows DSMC simulations to be applied to macroscopic engineering problems as well, and is not limited to simulations at the microscopic scale. Moreover, the DSMC method has been shown to converge to the solution of the Boltzmann equations, provided that some rules are respected in the numerical parameters, see Wagner [26]. The stochastic treatment has a price: the solution presents some inherent statistical noise, that can be reduced by suitable sampling time.

From the numerical point of view, the domain is divided in cells that are used to recognize neighboring particles, among which collisions are to be performed. In order for the solution to be physically meaningful, the computational grid should be smaller than the particles mean free path. A common choice consists in taking the grid size as 1/2 or 1/4 of the estimated local mean free path. The number of simulated particles is then chosen to ensure that every grid contains an adequate number of particles (possibly bigger than 10 as a rule of thumb - for sure not smaller than 5). Finally, the timestep has to be chosen to be smaller than the mean time between collisions, a value of 1/2 or 1/4 being a good choice.

4.2 Collisions and energy exchange

A number of models are available for computing molecular collisions and are reviewed in [18]. Collisions are assumed to be binary, and the assumption is valid for dilute gases.

The most simple model is the Hard Sphere (HS) model, that assuming the particles are rigid spheres predicts a cross section $\sigma = \pi d_{12}^2$, with d_{12} being the average of the spheres diameters. This proves to be a quite rough model, not able to correctly reproduce properties of the gas such as the viscosity.

More advanced models have been proposed, such as the Variable Hard Sphere (VHS), introducing a dependency of the cross-section on the collision energy and thus allowing for a much better prediction of the variation of viscosity with respect to temperature. In this work, a further extension will be used, called Variable Soft Sphere (VSS) model, relaxing the isotropic scattering pattern intrinsic in the previous two models: the deflection angle is modeled as $\chi = 2 \cos^{-1}[(b/d)^{1/\alpha}]$. All the details can be found in [18].

Inelastic collisions and chemistry

Over the years, the DSMC method has been extended to model the energy exchange among energy levels as well as chemical reactions. A number of models were proposed, such as the Rough Sphere model for example. The most common choice is the Larsen-Borgnakke model¹, which is employed in this work also.

Regarding chemical reactions, two main possibilities are available today: the TCE model (total collision energy) and the QK (quantum-kinetic) see Bird [27]. This work is based on the first.

Ambipolar assumption

As was discussed in Section 3, low density plasmas in absence of external electromagnetic fields can be modeled using the *ambipolar assumption*. This assumption is particularly needed in the field of DSMC, in fact due to the much smaller mass of electrons with respect to heavy particles, their velocity is much higher: in order to correctly track them, a correct timestep should be reduced by orders of magnitude.

In the ambipolar assumption, electrons are moved with their parent ions during the translation step and their energy is used only in computing the effect of collisions.

¹Although unrelated to the Larsen-Borgnakke model, the name of the Lagrangian solver developed in this work was chosen in honor of Larsen, due to the solver capacity of refining a solution from the point of view of the internal energy.

4.3 The SPARTA code

An open-source implementation of the DSMC method is provided by the SPARTA code -Stochastic PArallel Rarefied-gas Time-accurate Analyzer, developed at Sandia Laboratories [28]. Such solver implements the models introduced in the previous sections and will be used in this work.

The code gives to the user the possibility of obtaining a number of different outputs, computed from the properties of the particles. In Chapter 6 the code will be used to simulate the air flow around a meteoroid and a number of fields will be obtained, such as the velocity, temperature, density field and concentration of chemical species.

It is important to highlight a major deficiency of the SPARTA code: as is common for DSMC software, SPARTA is currently able to treat only reactions originating from binary reactions (such as $N_2 + O \rightarrow NO + N$) or three body dissociation reactions (for example $N_2 + O_2 \rightarrow N + N + O_2$). Recently, the possibility of computing recombination reactions was modeled, but such feature is not available for free electrons. This deficiency will be determinant in the study of free electrons in meteor trails and will lead to the necessity of a chemical correction.

Before moving to the actual simulations performed in this work, some training was performed: simple testcases were simulated and the results were verified to follow literature results. In the next section, the results of a simulation performed with SPARTA are reported.

4.4 Testcase: hypersonic rarefied flow over a sphere

As a proof of the capabilities of the DSMC method and of the SPARTA code, some results of an hypersonic simulation will be shown in this section. The analyzed testcase is the same that will be thoroughly discussed in Chapter 6 and represents a meteoroid during its atmospheric entry, but the attention in this section is focused not on the trail but towards the head region. In particular, the post-shock region is analyzed in terms of distribution function. The simulated sphere has a diameter of 1 cm and is moving at a velocity of 20 km/s at an altitude of 70 km. The flow is rarefied and shows a Knudsen number equal to 0.1.

A representation of the resulting temperature field is given in Fig. 4.1. The raise in the shock region is clearly visible, and the shock is very diffuse due to the rarefaction conditions.



Figure 4.1: Temperature field computed by SPARTA.

What is more interesting is that since the method provides solutions of the Boltzmann equations, out of equilibrium flows can be effectively simulated. In particular, at the simulated rarefied conditions the flow in the shock layer of the meteor is known to be *strongly* out of equilibrium. This fact can be appreciated if the distribution of the particles velocities is plotted (Fig. 4.2). The blue curve represents the distribution of longitudinal velocities, while the red curve is the distribution of transverse (radial) velocities.

While an equilibrium solution would present a distribution of velocity shaped as a Gaussian distribution (actually, a Maxwellian, see Chapter 2), the shown result can be seen to have a totally different shape. In particular, the various families of particles can be clearly distinguished. First of all, molecules are reaching the body from the left and have a positive velocity equal to the freestream value of 20 km/s: those particles can clearly be seen as the peak on the positive values of the velocity axis (blue curve). It is known that the temperature is linked to how much the distribution function is spread: the considered blue peak is quite narrow - the freestream particles are in fact at low temperature.

When the particles reach the wall, they heat up at the wall temperature (2000 K in this simulation) and bounce back in the other direction. Those particles can clearly be seen on the negative region of the axis and their temperature is seen to be higher than before. The two families are connected in the middle: this effect may be attributed to the few but still present collisions.

Finally, the curves are seen to superimpose on the red curves, showing that the vertical velocity distribution is as well the sum of two populations: a cold freestream population and a hotter one coming from the wall.

Since the DSMC software computes the temperature as a measure of how much the distribution function is spread (assumption valid in the equilibrium case only), it is possible to understand that this value does not have a physical meaning. This temperature should be identified more as a *geometrical* temperature.



Figure 4.2: Populations of particles in the shock layer.

Chapter 5

Development of a Lagrangian solver for detailed chemistry

The bulk of the time spent in this project consisted in the development of a solver able to *reprocess* simple flow simulations by introducing *arbitrarily complicated* chemical models. As a final result, a numerical implementation have been produced, able to treat 2D axisymmetric flows. The path to the creation of such solver will be detailed in this chapter. In Chapter 6, the solver will be applied to the study of meteor trails, allowing to obtain a description of the free electrons evolution, final goal of this work.

5.1 Rationale

The motivation for creating a solver able to reprocess an existing simulation is to be found in the practical difficulty of performing numerical simulations with very elaborated chemical models. In fact, if chemical reactions are to be taken into account, the set of governing equations grows in size: one mass conservation equation has to be added for each chemical species, as can be seen in equation 2.7.

The number of chemical species to be simulated if often very big: in hypersonic flows modeling for example, air is typically modeled as an 11 species mixture (and sometimes more). In many instances the number of species to be simulated is even higher: it's for example the case of meteor trails, where air species mix with ablated species coming from the meteoroid and chemical reactions produce additional species such as metallic oxides.

Chemically reactive flows are not the only situation where this practical issue arises: recent accurate ways of modeling high temperature flows out of equilibrium consist in modeling internal energy levels of atoms and molecules as *pseudo-species* and the exchange of energy among them as *pseudo-reactions*. Such approach is referred to as "state to state" modeling and promises extreme accuracy in terms of physical modeling, at the price of simulating a huge number of pseudo-species, in the order of 1000.

The idea underlying this work is the following: while a direct solution of the complete chemical problem is often impossible to obtain for practical reasons, it's possible to compute an initial rough solution and then refine it *a posteriori*. The suggested approach is based on three steps:

- 1. A baseline simulation including a simple chemical model is performed (with whatever numerical tool);
- 2. Streamlines are extracted from such solution;
- 3. An ad hoc solver is run over the streamlines, introducing a posteriori a (much) more detailed chemical model.

We refer to this approach as *Lagrangian* due to its streamline-marching nature. The key point in this approach is that the heavyweight nature of the multi-species problem will be balanced by an inherently lightweight Lagrangian formulation, allowing for *very* complicated chemical models to be taken into account. In the rest of this work, this ad hoc solver will be referred to as "Lagrangian reactor" or "Lagrangian solver".

Of course, the suggested approach is just an *approximation* to the real problem. In fact, this can be seen as a one-way coupling and no feedback of the refined results is provided on the starting solution, but the approach is seen to provide valuable results, at least for the performed testcases.

Lagrangian reactor and meteor trails

Due to the capability of refining an initial solution by adding a more elaborate set of reactions, this approach proves to be particularly suited for the current work, where the available method for computing the fluid dynamics of meteor trails is not able to realistically treat the chemistry of electrons. Moreover, the lightweight nature of this approach will enable to obtain a solution for very elongated trails, reaching some kilometers of size.

5.2 Lagrangian formulation of fluid equations

The first step towards the creation of the a reactor able to reprocess the solution along given streamlines is rewriting the governing equations from the Eulerian to the Lagrangian formulation. The developed solver will take the velocity and density fields¹ as given from the baseline solution and recompute the following:

- i) One mass conservation equation for each chemical species;
- ii) The total energy conservation equation.

¹The fact that the density field is taken *as it is* is a direct consequence of the fact that the velocity field is given. In fact, if the velocity field is not recomputed, there is no point in solving the mixture mass conservation equation, that would simply provide the same value as the previously computed, for the density.

In order to write the equations in the Lagrangian formulation for steady flows, the derivative along the streamline is expressed:

$$\boldsymbol{u} \cdot \boldsymbol{\nabla} \bullet = U \frac{\mathrm{d} \bullet}{\mathrm{d} s} \tag{5.1}$$

where \boldsymbol{u} is the flowfield velocity vector, U its module and s is the streamline curvilinear abscissa. The result of such procedure are shown in the following, where also the mass fraction $Y_i = \rho_i / \rho$ was introduced. Equations are formulated and solved in the steady state conditions.

An important remark on the trail geometry allows to obtain important simplifications in the nature of the equations. Due to the extremely slender nature of meteor trails, diffusion terms can be evaluated only radially. Longitudinal diffusion will thus be neglected with respect to the radial one: this approximation is justified based on the disparity of the radial and longitudinal gradients).

Mass conservation for chemical species

$$\frac{\mathrm{d}Y_i}{\mathrm{d}s} = \frac{\dot{\omega}_i - \boldsymbol{\nabla} \cdot \left(\rho_i \boldsymbol{V}_i^d\right)}{\rho U} \tag{5.2}$$

As said, the diffusive mass flux will be evaluated only in the radial direction.

Temperature equation

An equation for the temperature is obtained starting from the enthalpy equation, formulated along a streamline, in the steady state case:

$$\frac{\mathrm{d}H}{\mathrm{d}s} = \frac{\boldsymbol{\nabla} \cdot (\boldsymbol{u} \cdot \boldsymbol{\tau}) - \boldsymbol{\nabla} \cdot \boldsymbol{q}}{\rho U} = \frac{\mathcal{Q}}{\rho U}$$
(5.3)

By expanding the total enthalpy per unit mass H into its internal contribution h and kinetic contribution $U^2/2$, and recalling that for a perfect gas, $h = c_p T$, an equation for the evolution of the temperature along the streamline is found:

$$\frac{\mathrm{d}T}{\mathrm{d}s} = \frac{1}{U} \left[\frac{\mathcal{Q}}{\rho} - U \frac{\mathrm{d}U^2/2}{\mathrm{d}t} - \sum_{i \in \mathcal{S}} \frac{h_i \dot{\omega}_i}{\rho} \right] \Big/ \left[\sum_{i \in \mathcal{S}} Y_i c_{p,i} \right]$$
(5.4)

where c_p are the specific heats per unit mass. The Lagrangian reactor can take the value of Q from the baseline simulation: in this case, the energy variation among to subsequent streamline points is directly extracted from the baseline simulation and no assumption needs to be done on the fluxes. This implies that the solver operating in this mode is potentially able to recompute even rarefied solutions.

If the reactor is asked to recompute Q, this will be done by computing the heat flux only in the vertical direction, possible assumption due to the slenderness of the trail. Also, if Q is to be computed, the Lagrangian reactor will neglect the power of viscous forces, in the hypothesis that the flow in the trail is almost uniform (Chapter 6 will show that this is the case).

Mathematical nature of the equations

The governing equations for the Lagrangian solver have a parabolic nature due to the hypothesis that fluxes are only directed radially. This fact legitimates the employment of a marching method such as the Lagrangian software developed in this work. A marching approach is notoriously much lighter than full multidimentional CFD simulations.

5.3 The LARSEN code

The work on a Lagrangian reactor able to correct the chemistry of a baseline simulation was started at VKI by the author before the beginning of the this project. A version of the described Lagrangian solver was in fact recently developed and is described in [29]. Such solver is named LARSEN, standing for LAgrangian Reactor for StrEams in Nonequilibrium.

The formulation of the LARSEN code prior to the current work was single-streamline. For this reason, the code was not suitable for an application to the determination of free electrons in meteor trails, since diffusion of electrons from one streamline to the neighboring one could in no way be computed.

This work focused on the extension of the LARSEN code to a multi-streamlines formulation. Multiple streamlines are imported from the baseline solution and governing equations are solved *simultaneously* along all of them. Diffusion fluxes are then computed using an implicit approach.

Software details

The LARSEN code is implemented in C++ in an object-oriented fashion. Thermodynamic and transport properties, as well as chemical reactions, are obtained using the Mutation++ library developed at VKI. The integration of governing equations is performed using the boost libraries and the solution is exported using the VTK libraries, for an easy analysis with graphical software such as ParaView.

It should be stressed that **all** the used libraries are open-source, and the software for analyzing the solution is open-source as well. For this reason, the code suffers from no license issues.

5.4 One-way refinement approach

As explained, the "Lagrangian approach" for thermochemical refinement is basically a convenient *approximation* of the problem. As such, it's important to understand whether this approximation actually leads to improved results or not.

This answer is partially given in [29], where a number of testcases is analyzed. The performed testcases regard the thermochemical relaxation past a shockwave: first, a baseline simulation is computed using a simple chemical model; this solution is then fed to the LARSEN solver and a refined solution is computed, adding many more chemical

species; finally, results are compared to a third complete simulation, obtained by taking into account all the species from the beginning.

In all the testcases performed the results from the Lagrangian reactor are seen to be a *significant improvement* to the baseline solution: the error with respect to the full solution was reduced *at least* by the 50%, in many cases much more. An example extracted from [29] is provided in Fig. 5.1: the Lagrangian reactor is asked to recompute the thermal relaxation of an air mixture by adding the possibility of ionization. The solution is found to be very close to the exact solution in terms of temperature, with some deviations in the transitory region. Values for chemical species are found to be in good agreement and almost exact at the equilibrium, even for ionized species, that were not present in the initial baseline simulation.



Figure 5.1: Correction of a baseline solution with LARSEN.

An additional verification of the approach is obtained in Chapter 6, where the Lagrangian simulation is found to provide results that are *very close* to the baseline simulation in terms of free electrons diffusion.

Those results suggest that the proposed one-way coupling can actually be used to improve the chemistry in baseline simulations.

5.5 Implementation of diffusion fluxes

The main contribution of this work to the LARSEN software lies in the implementation of diffusion fluxes (of mass and energy). Those terms appear as derivatives along the radial direction², the equations thus become a set of PDEs and additional efforts are required for their solution with respect to the original version of LARSEN. Two main modifications have thus been implemented:

• A finite volume approach is introduced in the transverse direction, to evaluate diffusion fluxes across streamlines;

 $^{^{2}}$ As explained, the longitudinal component of mass fluxes is here neglected: the slender nature of the trail ensures that the gradients are mainly in the transverse direction.
• The integration process is performed along the trail axis, simultaneously for all the streamlines.

The numerical solution of the governing equations is treated in detail in the next sections.

5.5.1 Finite volumes for diffusion fluxes

During the integration process along the streamlines, the right hand sides of equations 5.4 and 5.2 need to be evaluated at each integration step. Terms such as the chemical production rates $\dot{\omega}_i$, the enthalpies h_i and specific heats $c_{p,i}$ are easily evaluated since they only depend on the local state along the streamline. On the other hand the diffusion terms need to take into account the temperature and species concentration gradients across neighboring streamlines. A 1D finite volume approach [30] is employed across the streamlines.



Figure 5.2: Finite volume approach across streamlines for the fluxes computation.

Finite volumes mesh

For a given integration location x_n , a cell is defined for each streamline, taking its interfaces halfway from the neighboring streamlines, as shown in Fig 5.2. The position of the interfaces for the *i*-th streamline is thus defined as:

$$y_{i+1/2} = \frac{y_{i+1} + y_i}{2} \qquad \qquad y_{i-1/2} = \frac{y_i + y_{i-1}}{2} \tag{5.5}$$

The interfaces position is used to find the geometrical cell center y_i^c , as well as the cell size Δy_i :

$$y_i^c = \frac{y_{i+1/2} + y_{i-1/2}}{2} \qquad \Delta y_i = y_{i+1/2} - y_{i-1/2} \tag{5.6}$$

It should be noted that the cell center is not necessarily located on the streamline: this is the case only if streamlines are uniformly spaced.

Diffusive fluxes

Once the finite volumes mesh has been defined, the divergence of diffusive fluxes can be computed from the flux values at the cell interfaces. By denoting with \mathcal{F}^d the diffusive mass or heat flux, the equation for the *i*-th cell reads:

$$\begin{cases} \left(\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}}^{d}\right)_{i} = \frac{\boldsymbol{\mathcal{F}}_{i+1/2}^{d} - \boldsymbol{\mathcal{F}}_{i-1/2}^{d}}{\Delta y_{i}} & \leftarrow \quad Cartesian \ case \\ \left(\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}}^{d}\right)_{i} = \frac{1}{r_{c}} \frac{\left(r\boldsymbol{\mathcal{F}}^{d}\right)_{i+1/2} - \left(r\boldsymbol{\mathcal{F}}^{d}\right)_{i-1/2}}{\Delta r_{i}} & \leftarrow \quad axisymmetric \ case \end{cases}$$
(5.7)

where Δy_i and Δr_i are the length of the *i*-th cell and r_c is the position of the cell center. The subscript $i \pm 1/2$ indicates that the term has to be evaluated respectively at the top or bottom interface and is detailed in the following.

The computation of both heat and mass fluxes requires the evaluation of transport properties of the gas mixture, respectively the thermal conductivity k and the diffusion coefficients D_{kl} . Those properties are evaluated at the interface, where the thermodynamic state is taken as the weighted average of the neighboring cells values, as done in [31]. By defining with p the integration variables (species mass fractions Y_i or temperature T), the value at the interface i + 1/2 and its gradient across the interface are computed as (similarly for the lower interface):

$$p_{i+1/2} = \frac{p_{i+1}\Delta y_{i+1} + p_i\Delta y_i}{\Delta y_{i+1} + \Delta y_i} \quad \text{and} \quad \left(\frac{\partial p}{\partial y}\right)_{i+1/2} = 2\left(\frac{p_{i+1} - p_i}{\Delta y_{i+1} + \Delta y_i}\right) \tag{5.8}$$

where Δy_{i+1} and Δy_i respectively denote the distance of the streamline i+1 and i from the considered interface. It should be noted that those expressions hold for both the 2D Cartesian and the axisymmetrical case.

Heat flux

The heat flux receives a particular treatment. In fact, the user can choose how to treat the term Q in equation 5.4. One possibility consists in importing it from the baseline simulation: in this case the software computes the variation of enthalpy among two successive points along the streamline and then computes Q accordingly:

$$\mathcal{Q} = \frac{\mathrm{D}H}{\mathrm{D}t} = U \frac{\mathrm{d}H}{\mathrm{d}s} \approx U \frac{\Delta H}{\Delta s}$$
 (5.9)

This treatment of the term Q corresponds in taking the energy fluxes from the baseline simulation. This is a trick that allows to avoid recomputing the energy fluxes, and allows a variation of enthalpy to occur even if one only streamline is analyzed. This feature was already implemented in the existing code before this work and the reader is referred to [29] for a deeper explanation. Another possibility, implemented during this work, consists in obtaining the heat flux using the Fourier's law, computing temperature gradients across the cell interfaces. In this case, the term Q is taken as:

$$\boldsymbol{\mathcal{Q}} = \boldsymbol{\nabla} \cdot \boldsymbol{q} \tag{5.10}$$

The heat flux is currently implemented via the Fourier law: $q = -k\nabla T + \sum_k \rho_k h_k V_k^d$. The flux at the interface $i \pm 1/2$ thus reads:

$$\mathcal{F}_{i\pm 1/2}^d \coloneqq q_{i\pm 1/2} = -k_{i\pm 1/2} \left(\frac{\partial T}{\partial y}\right)_{i\pm 1/2}$$
(5.11)

where the temperature gradient is evaluated using equation 5.8. The power of viscous forces is not yet implemented since the solver was conceived for studying quasi-uniform flows. However, its implementation is trivial and is suggested as a future work.

Mass fluxes

The evaluation of mass flux $J_k = \rho_i V_k^d$ for the species k needs computing the diffusion velocities V_k^d , obtained from the gradients of species concentration and the multispecies diffusion matrix D_{kl} :

$$J_k = \rho_k V_k^d = -\rho_k \sum_l D_{kl} \frac{\partial X_l}{\partial y} + \mathcal{K}_k \boldsymbol{E}$$
(5.12)

The evaluation at the interface of this flux is performed as done in equation 5.11. The gradient of mole fractions is currently the only driving force introduced. Other effects (barotropic diffusion and Soret effect) are suggested as a future development of the code.

Boundary cells

A particular treatment is reserved to the boundary cells. For symmetry reasons, the lower cell is supposed to have a zero flux from the bottom interface, while it can exchange mass and energy through the top. The upper cell on the other hand is supposed to have a total zero net flux: the flux on the overlying interface is set equal to the underlying one.

5.5.2 Integration along multiple streamlines

The introduction of mass and energy fluxes imply the need of computing the vertical gradients of species concentration and temperature in the vertical direction. This means that at a given timestep this information must be available: all the streamlines must have reached the same longitudinal position. On the other hand, if integration would be performed along the streamline, synchronization would be lost, the quicker streamlines leaving behind the slower ones. For this reason, the formulation is slightly modified in order to perform the integration along the x axis simultaneously for all the streamlines. This approach is done with a simple change of variables, introducing the local slope α .

$$dx = \cos \alpha \, ds \implies \frac{d \bullet}{dx} = \frac{1}{\cos \alpha} \frac{d \bullet}{ds}$$
 (5.13)

It should be noted that this requires the streamlines to be somehow aligned along the x axis. This is definitely the case for meteor trails, where streamlines are almost parallel. A scheme of the process is shown in Fig. 5.3.

In this way, the integration can be performed simultaneously for all the streamlines and the problem reduces to a system of equations:



Figure 5.3: Conversion from curvilinear abscissa to trail axis coordinate.

where ξ_i are the variables along the *i*-th streamline (mass fractions of chemical species and temperature). As an example, equation 5.15 shows the mass fraction of electrons on the *j*-th streamline.

Finally, the integration of the system of equations along the x direction is performed using a *rosenbrock* 4 method: a stiff solver is needed for correctly dealing with the chemical source term, that typically introduces a number of very different time scales into the system.

5.5.3 Verification of the code

The modifications done to the software LARSEN, detailed in the previous paragraphs, have been verified against simple testcases and provide confidence that the implementation procedure have been successful. In particular, a simple verification of the mass diffusion implementation is shown in this section: the solution provided by LARSEN was compared to the solution of the diffusion equation.

$$\frac{\partial U}{\partial x} = \alpha \frac{\partial^2 U}{\partial y^2} \tag{5.16}$$

The solution of equation 5.16 is known for the case of imposed values at the boundaries y = 0 and $y \to \infty$. The equation can be shown to be self-similar, the similarity variable being $\eta = y/\sqrt{4\alpha x}$, and the solution is given in terms of the *errorfunction*:

$$\theta = \operatorname{erf}(\eta) \quad \text{with} \quad \theta = \frac{U - U_0}{U_{\text{init}} - U_0}$$
(5.17)

The mass equation solved by the Lagrangian reactor LARSEN follows the simpler diffusion equation in case of small concentration perturbations. A perturbation of concentration is then applied to a binary mixture of molecular oxygen and nitrogen and the evolution along x is seen to match the theoretical prediction to a very good accuracy.



Figure 5.4: Diffusion: analytical solution erf vs value computed by LARSEN.

Other than this 2D case, verification was performed for the axisymmetric case as well, for both mass and energy diffusion. Since the analytical solution for the axisymmetric case is significantly more complicated, a numerical result was used as comparison. In all the cases, the solution of LARSEN is seen to follow closely the reference solutions.

Validation of the code against experimental results has not been performed so far due to the difficulties in obtaining reliable reference data for flight conditions typical of meteoric flows. However, a big amount of data is available at VKI for the Plasmatron jet for the continuum regime: a comparison of the developed took with the freestream plasma jet is suggested as a possible future work activity.

Finally, an *a posteriori* verification will be found in Chapter 6, where the solution of the Lagrangian reactor will be found to closely follow the diffusion profile predicted via the DSMC solver.

Chapter 6

Results

In the previous chapters, the physical and numerical background for the study of atmospheric entry plasma flows was discussed and a new method based on a Lagrangian approach was introduced. All those theories, models and tools converge in this chapter, where the aim of this work is finally met, namely the simulation of free electrons in meteor trails.

The goal of this chapter is establishing a methodology for analyzing meteor trails. Attention focuses on a simple testcase, a nonablating meteoroid simulated at one point of its atmospheric entry trajectory. Results shown in this chapter are thus to be intended as a starting point for a more extended analysis performed on different meteor sizes and flight conditions, possibly taking into account ablated species as well.

The studied testcase consists in a meteoroid of 1 cm diameter, entering the Earth's atmosphere at a velocity of 20 km/s. The simulation is carried out at an altitude of approximately 70 km from the ground, that given the size of the meteoroid gives rise to a big Knudsen number and the flow is thus rarefied. Table 6.1 resumes the current testcase characteristics, together with the Knudsen and Mach numbers, while a picture extracted from the DSMC simulation is shown in Fig. 6.1.



Table 6.1: Size and flight conditionsfor the simulated meteoroid.

Figure 6.1: Extract from DSMC simulation.

First of all, in Section 6.1 the rarefied flowfield will be studied using the Direct Simulation Monte Carlo method, introduced in Chapter 4. The method will provide a good knowledge of the flowfield in the trail, as well as a first estimation of the free electrons concentration.

In Section 6.2, the meteor will be analyzed from the fluid dynamics point of view: the main phenomena will be highlighted and three different regions will be identified, where the flowfield shows different features.

Due to the limitations on recombination processes and complex chemical mechanisms in the DSMC algorithm, the prediction of electron concentration obtained in Section 6.1 cannot be relied upon. For this reason, in Section 6.4 the DSMC solution will be postprocessed using the Lagrangian reactor developed in this work, providing a more reliable map of free electrons concentration. Finally, the Lagrangian reactor will be also used to study the electron concentration up to a distance of 2 km from the meteoroid.

6.1 Meteor simulations at high altitude

The first step in the current analysis of meteor trails consists in performing a DSMC simulation of a nonablating meteor in air, with the open-source software SPARTA (Section 4.3). The meteoroid is approximated as a sphere of 1 cm diameter and the air gas mixture is initially entirely composed by diatomic nitrogen an oxygen, eventually chemically reacting and dissociating near the body. The initial air composition in mole fraction is 0.791 parts of N_2 and 0.209 parts of O_2 . The enabled set of chemical reactions may lead to the production of an additional number of species, namely N, O, NO, N^+ , O^+ , N_2^+ , O_2^+ , NO^+ and free electrons e^- . The total number of chemical species is thus 11, and this model will accordingly be referred to as "air 11". Reaction rates are taken from Park [25]. Freestream conditions for the simulated trajectory point are given in table 6.2.

$$\begin{array}{c|c|c} U_{\infty} & 20\,000 \text{ m/s} \\ n_{\infty} & 1.19 \times 10^{21} \text{ part/m}^3 \\ \rho_{\infty} & 5.69 \times 10^{-5} \text{ kg/m}^3 \\ T_{\infty} & 220 \text{ K} \\ T_{wall} & 2000 \text{ K} \end{array}$$

Table 6.2: Free stream conditions for DSMC simulation.

Collisions among molecules are computed using the VSS model and the relaxation of internal energy is modeled through the Larsen-Borgnakke method, as discussed in Chapter 4. Collisions of molecules with the meteoroid surface are treated as fully diffusive (accommodation coefficient equal to 1).

The choice of the wall temperature is an important parameter for the study of the stagnation point region, where a big number of free electrons are produced. The wall temperature T_{wall} is taken to be equal to 2000 K, that would be a realistic value for a melting meteoroid composed of rock or iron. It's important to stress that despite this choice for the wall temperature, in this simulation the meteoroid *does not ablate*. Ablated

species would have a number of effects, including modifying the flowfield and the electrons concentration. However, the real goal of this chapter is developing a methodology for the trail study: more accurate simulations may be performed in the future to increase the physical realm of the model.

6.1.1 Grid and numerical details

The performed simulation is 2D axisymmetric and the domain is a box with the lower side coincident to the meteor trail, as shown in Fig. 6.2. Particles are injected at the inlet boundary at freestream conditions and when they cross the outlet boundary they are removed from the computational domain. The lower side, coincident to the trail axis, is modeled as fully reflective to introduce axial symmetry. At the upper boundary, as for the inlet, particles are seeded during the simulation at freestream velocity, and are eventually pushed out of the domain by collisions with inner particles.



Figure 6.2: Computational domain for the DSMC simulation.

The appropriate choice of parameters for DSMC simulations is discussed in Chapter 4; the main parameters are here briefly reviewed. The timestep for the simulation was chosen to ensure that everywhere in the domain its value is smaller than the mean time between collisions and is specified in table 6.3. This constraint is particularly heavy in the post-shock region, where the high values of temperature and density are higher than freestream ones by orders of magnitude. The parameter F_{num} , ratio between real and simulated particles is shown in the same table and was chosen to ensure that each cell contains in average 20 particles.

timestep
$$\Delta t \mid 4.5 \times 10^{-9} \text{ s}$$

 $F_{num} \mid 4 \times 10^{16}$
 $\frac{N_{cells} \mid N_{particles}}{2\,300\,000 \mid 15\,000\,000}$

Table 6.3: DSMC simulation: parameters.

Table 6.4: DSMC simulation: number of cells and simulated particles.

The grid cells are chosen to have a size which is *smaller* than the mean free path. Dimensions for the asymptotic grid cells are given in table 6.3. Again, the most critical



Figure 6.3: DSMC simulation: detail of the grid near the meteoroid.





region is the post-shock region, since at higher densities the mean free path reduces and the grid must correspondingly be reduced. Three levels of grid refinement were adopted, shown in Fig. 6.3.

The trail of high velocity rarefied flows is notoriously hard to simulate in a rigorous way, due to the difficulty of having an adequate number of simulated particles in the shadow of the body. Fig. 6.4 illustrates this problem, showing that the cells near the rear stagnation point have a number of cells below 5, absolute minimum number to obtain statistically significative results.¹ From the point of view of the trail analysis this is not an issue, since the situation improves very quickly as the trail develops.

The simulation is run until the number of simulated particles settles to a final value. Once this value becomes steady, the transitory part of the simulation is finished and running averages are started over the particles properties. This will provide macroscopic flow properties such as the velocity, density and temperature of the obtained *steady state solution*.

Since the simulated domain is very slender, a domain sensitivity analysis was performed: another simulation was run on a wider domain (twice as big in the vertical direction) but no difference was found on the results. In fact, the advection velocity is much higher than the velocity of propagation of disturbances in the transverse direction, since the flow is highly hypersonic.

6.1.2 Simulation results

The solution obtained with the SPARTA program is given in terms of a number of fields. Among those, the most useful from the fluid dynamics point of view are:

- Velocity field (u, v);
- Number density field (particles per unit volume);
- Translational, rotational and vibrational temperatures;
- Number density of each chemical species.

¹This is a commonly adopted rule-of-thumb, discussed in Chapter 4

Among the chemical species, the free electrons number density is provided, of particular interest for this work. Fig. 6.5 shows the temperature, velocity and number density fields.



Figure 6.5: DSMC simulation: temperature, velocity and number density fields.

Those results are very interesting from the fluid dynamics point of view. From the temperature plot in particular, the shock layer is clearly visible in front of the body. The temperature raises to *extremely* high values: in fact this point is found to be highly out of equilibrium, as was already discussed in Section 4.4, where a geometrical temperature was introduced.

Another very interesting fact shown in Section 4.4 is the diffused nature of the shock. This is a characteristic result of rarefied fluid dynamics: shock waves become more and more spread as the Knudsen number increases. In fact, the shockwave thickness is in the order of the molecular mean free path, comparable to the body size in high Knudsen number flows.

The shape of the bow-shock is clearly visible by the density plot, highlighted by an increase in the density. Again, the shock results very diffuse and the increase in the flow variables is thus smooth.

Finally, attention should be put to the trail region, where the density shows to be quite low with respect to the freestream values. The flow, compressed at the stagnation point region, expands on the sides of the meteoroid and due to the extremely high velocity takes a big amount of time to fill the trail, as will be further discussed in the next sections. For reasons to be explained, this trail property will need to be carefully taken into account for the free electrons analysis.

Starting from the temperature and density fields, the pressure field can be obtained with the perfect gas law (at thermal equilibrium the electron temperature T_e is equal to the heavy species temperature T_h):

$$P = n k_B T \tag{6.1}$$

where n is the particles number density, k_B is the Boltzmann constant and T the mixture translational temperature. The freestream pressure is found to be equal to: $P_{\infty} = 3.61$ Pa. Inspecting the pressure plot, given in Fig. 6.6 the compression of the gas at the stagnation point can be clearly seen. The raise in pressure in this region amounts to four orders of magnitude.



Figure 6.6: DSMC simulation: pressure field.

Regarding the trail region, the plot reveals that very early the pressure drops back to low values, characteristic of the free stream. This has an important consequence in terms of physical modeling: the role of radiation may play an important part in the energy balance². Those effects are treated in [32]. However, those effects are here totally neglected, which is a common practice in DSMC simulations. In the next sections a the Lagrangian reactor here developed will be applied to correct the current DSMC simulation: this software may in the future be used to introduce those *collisional-radiative* effects as well, but this is out of the scope of this work.

One more field deserves our attention: the number density of free electrons (number of free electrons per unit volume), shown in Fig. 6.7.



Figure 6.7: DSMC simulation: number density of free electrons [particles/ m^3].

Electrons are mainly produced in the shock layer region, and are advected around the meteoroid and transported in the trail. If the numerical value of the number density is analyzed, its value is found to be very high. In particular, at those values of concentrations for free electrons, incoming radio waves would be *totally reflected* by the trail [33]. This result is simply the numerical confirmation that this kind of hypersonic bodies can actually be observed using radio techniques.

The number density of free electrons is seen to gradually decrease as the trail develops, as a result of mass diffusion processes. Highly concentrated free electrons around the body diffuse in the surroundings and the dimension of the ionized region increases along the x axis. While analyzing the effect of diffusion, that conserves the total number of

²Such effects appear to be important for air at pressures below 1000 Pa.

electrons but spreads them in the surrounding, it should be recalled that the simulation is axisymmetric, the effect is thus stronger with respect to 2D Cartesian geometries. Despite the effect of diffusion, the free electrons concentration is seen to be very high even at the exit of the computational domain: according to those results the portion of the trail taking part to the radio waves reflection exceeds the computational domain.

One very important observation has to be made at this point, regarding the shown results. As was explained in Chapter 4, the DSMC method currently suffers from an important limitation: **recombination of free electrons is not computed**. During the simulation, particles collide with each other and some of those collisions result in the production of free electrons, but the opposite reaction - recombination of free electrons with ions - is not taken into account.

This fact implies that the performed DSMC simulation³ while reliable from the point of view of velocity and density fields,⁴ should not be trusted a priori in terms of electrons concentrations. The Lagrangian reactor developed in this work provides a possible solution to this problem. In fact, in the next sections that approach will be employed to *reprocess* the current DSMC simulation and will provide the sought map of free electrons along the trail, taking into account both diffusion and recombination processes.

Simulations at different flight velocity

In order to give an idea of what happens to meteors entering the atmosphere at higher velocity, some simulations were performed for meteors at higher velocities. An increased speed results in mainly three effects: the maximum temperature increases, the amount of electrons produced increases as well and finally the trail gets more rarefied and persistent.

The current simulation will be compared to a 72 km/s simulation in Appendix A.2 and a comparison with the 20 km/s results is provided in terms of temperature and density fields.

Statistical analysis of the flow field

As discussed in Chapter 4, the DSMC method is a stochastic way of solving the Boltzmann equation. As such, the information carried in the DSMC solution is not limited to the temperature, velocity and density fields, but is much richer: the DSMC method provides an estimation of the velocity distribution function, carrying information on the microscopic state of the gas in each point of the domain.

An interesting analysis of the trail can be thus performed from the statistical point of view. Results of such analysis are reported in Appendix B.

An important result of such analysis needs to be here highlighted: although in rarefied conditions, the particles velocity distribution is seen to be very close to a Maxwellian, the deviation decreasing quickly as the trail develops. This fact implies that despite the degree of rarefaction is high, a solution from the Lagrangian solver - based on continuum hypothesis - applies as well.

³At least in the current implementation, that does not include recombination reactions.

⁴This statement will be discussed in Section 6.2.

6.2 Fluid dynamics analysis of the trail

Some important observations can be made from the DSMC results, allowing for an understanding of the fluid dynamics of the trail. From Fig. 6.5, the temperature and velocity fields appear to reach the freestream conditions quickly as the trail develops, while the density seems to require much more time. This is confirmed by inspecting the flowfield quantities along the trail axis, shown in Fig. 6.8.



Figure 6.8: Flowfield quantities along the trail axis.

The behavior of density requires further investigation: despite temperature and velocity monotonically approach the freestream conditions, density initially increases towards the freestream value of 5.69×10^{-5} kg/m3, but around 30 diameters from the body decreases again. This observation is crucial for the study of elementary processes in the trail: a longer domain is required if a detailed solution is sought in terms of chemistry.

Cross sections at various locations along the trail axis were extracted from the DSMC simulation and results are shown in Fig. 6.9. The first line (green) is located at x = 0.025 m, while the last one (red) is located at x = 0.2 m. The trail size is clearly visible from the first line in the density plot: the density starts very low at the axis, raises through the diffuse shock layer (see Fig. 6.5) and finally reaches freestream values at a radial position r = 0.03 m. Marching along the trail, the density profile is advected outwards: this is due to a vertical velocity component of the streamlines (Fig. 6.9). This component eventually vanishes, and the behavior is expected to reverse at a certain point along the trail: streamlines are likely to converge again towards the trail axis, until the density will finally reach the freestream values. The behavior of density in the field is thus explained by the vertical component of the velocity. An analysis of the streamlines is given in Appendix A.1, where the density behavior is explained graphically.



Figure 6.9: Velocity components and density at cross sections along the trail.

Fluid dynamic regions composing a meteor

From what was discussed in the preceding paragraphs, it's possible to decompose the meteor phenomenon in three regions showing different fluid dynamic features:

- **Region i)**: first of all we have the front region. Near the body a strong shockwave develops, the temperature raises and a big quantity of free electrons are produced and advected to the next region.
- **Region ii**): the trail starts developing and the temperature, velocity and density gradually approach freestream values. This region was partially simulated and analyzed in this work.
- **Region iii)**: finally, flow quantities reach freestream values. At this point electrons are expected to still be present: if so, they keep diffusing in the surrounding and reacting until their concentration completely vanishes.

The DSMC solution deeply analyzed in the previous sections don't take recombination reactions into account. One question arises: would the flow features change if recombination is taken into account? Fortunately, it's not the case. Recombination reactions are exothermic and would clearly change the temperature field, however as shown in Appendix A.3, the role played by chemistry quickly becomes marginal from the flow field point of view as the trail develops.

Although apparently disconnected from the quest for electrons in the meteor trail, the trail flow properties discussed in this section will have important consequences in the solution strategy adopted in the next sections.

6.3 Intermediate conclusions: need for an alternate approach

A number of results were obtained in the previous sections. The meteor trail was simulated using a DSMC approach and a solution for the free electrons concentration was obtained. Such result predicts a large number of electrons in the trail, able to totally reflect radio signals sent by meteor detection stations. In particular, the predicted ionization degree is so high that even at the exit of the simulated domain the trail seems able to totally reflect radio signals.

Issue 1: no recombination

The shown results are however affected by a strong limitation: the employed DSMC method is not able to compute recombination reactions, so that a fundamental mechanism in the evolution of free electrons is missing. This *might* be the reason why the predicted ionization degree is so high, further investigation is thus required.

Issue 2: huge computational domain

The "recombination issue" is just *one* Achilles' heel of the DSMC approach. A second disadvantage arises: if the ionized portion of the trail would be much longer than the currently simulated distance, as the previous simulations seems to suggest, additional simulations would need to be performed, this time on a vastly longer domain - which would imply prohibitive computational times.

VKI's answer to the problem

In the next section, the Lagrangian approach developed in this work will provide an answer to those issues. The computed DSMC results will be used as a baseline simulation and fed to the Lagrangian reactor, that will recompute the concentration of chemical species, this time including recombination among the reactions.

The application of the Lagrangian reactor is legitimated by a number of results obtained in the previous sections. In particular, it should be noted that:

- Streamlines are found to be almost parallel and well aligned to the symmetry axis $(v \ll u, \text{ see also Appendix A.1})$. The *x*-integration marching approach is thus applicable;
- The analysis of the particles' velocity distribution reveals that the population is Maxwellian to a good approximation. The Lagrangian approach, that introduces diffusion properties based on continuum assumptions, can thus be applied.

The following sections will proceed as follows:

- 1. The Lagrangian reactor will be applied to recomputing the electron density from the DSMC simulation, tackling the first region of the trail, defined "region (ii)";
- 2. The residual electrons concentration will be found to be still very high at the exit of the computational domain. The Lagrangian reactor will then be applied to region (iii) and the electron density will be determined for a length of 2 km.

It is interesting to remark that the study of the ionization in region (ii) of the trail is fundamentally novel in the meteoric field. The common approach in fact models the whole trail as if it was directly in the freestream conditions. Since the ionized trail is extremely long (some km), an accurate description of region (ii) may seem just an academic exercise, but it's not the case: in fact, it will be shown that around the 30% of electrons recombine in this region. The determination of the number of electrons that survive region (ii) and keep evolving along the trail is thus to be obtained by taking into account the detailed structure of region (ii), where lower density zones are present, as well as overshoots. Those effects are automatically taken into account with the simulations performed in the next sections.

6.4 Lagrangian simulations of meteor trails

In the last part of this report, the Lagrangian reactor developed in this work will be applied to the study of the free electrons concentration in meteor trails. The final result will be a map of electrons number density up to a distance of 2 km.

As seen in Section 6.2, the meteor phenomenon can be divided from the fluid dynamics point of view in three regions, schematically shown in Fig. 6.10:

- **Region i)**: near the meteoroid a strong shockwave develops, temperature raises and the bulk of free electrons is produced.
- **Region ii**): after the meteoroid, the trail development begins and flow quantities such as density and velocity approach the free-stream values.
- **Region iii)**: in the (very long) remaining part of the trail the flowfield is almost uniform and residual free electrons diffuse and recombine with ions.



Figure 6.10: Fluid dynamic regions in meteoric flow. Drawing not in scale.

A DSMC solution was obtained for region (ii) but was lacking in terms of chemical modeling since recombination of free electrons was not computed. The first step of this chapter will consist in recomputing the concentration of chemical species in this region using the Lagrangian reactor. A map of free electrons will be obtained in region (ii). Finally, the evolution of electrons surviving region (ii) will be studied in region (iii), up to a distance of 2 km.

It should be noted that the supersonic nature of the flow ensures that information does not travel backwards⁵. As a result, each section of the trail can be treated separately, with initial conditions taken from the exit of the previous one.

6.4.1 Lagrangian reactor in the close-region

As explained in Chapter 5, the idea behind the Lagrangian reactor consists in starting from a baseline simulation, extracting the velocity and density fields and recomputing the remaining quantities: temperature and concentration of chemical species. The procedure for correcting the DSMC simulation is composed by two steps:

- 1. Streamlines are extracted from the DSMC simulation in terms of velocity, density, temperature and concentration of species;
- 2. The streamlines are fed to the Lagrangian solver LARSEN, that returns an improved map of chemical species and temperature.

The computational domain is shown in Fig. 6.11 and is taken from the DSMC simulation, starting from 2 diameters after the meteoroid surface and extending to 35 diameters from the meteoroid. The domain is seen to follow streamlines.



Figure 6.11: Domain for the Lagrangian refinement of region (ii). Meteoroid not in scale.

It should be stressed that the Lagrangian solver takes the *initial* temperature and chemical species composition from the *beginning* of the streamlines, that is from the inlet of the DSMC computational domain. The starting composition is thus the same as for DSMC simulations, while the evolution may change according to the models enabled.

In this section of the trail the velocity field changes considerably. The enthalpy variation along the streamline is thus taken externally, as discussed in Chapter 5.

As a final note, while the DSMC simulation is inherently multi-temperature, the current implementation of the Lagrangian solver LARSEN assumes thermal equilibrium. The development of a $T-T_v$ version of the solver is suggested as a future activity.

⁵As long as diffusion processes are neglected in the streaming direction. This is the case in the current problem.

Direct comparison with DSMC: no recombination

As a preliminary attempt, the Lagrangian solver was applied to the DSMC solution by *switching off recombination reactions*. In this way the solver mimics the DSMC solution, where no recombination occurs and the electrons concentration decreases only due to diffusion processes. The free electrons density was then extracted at the exit of the domain (x = 0.35m) in the radial direction and is shown in Fig. 6.12.



Figure 6.12: Number density of free electrons at the exit of computational domain. Chemical reactions switched off.

As can be seen, results from DSMC and Lagrangian solver are surprisingly close to each other although:

- The DSMC method is a particle-based method, while the Lagrangian solver is continuum-based: transport properties are computed using different models;
- The trail is rarefied and partly out of equilibrium (as discussed in Appendix B)⁶

Due to the capability of reproducing DSMC results, the Lagrangian solver is believed to provide a reliable solution in terms of electrons diffusion. It should be noted that as the trail develops, the particles tend to reach thermodynamic equilibrium and the continuum solution is expected to become more and more precise.

Diffusion vs recombination effects

In the introduction, an analysis of the third Damköhler parameter suggested that the effects of diffusion could be estimated to be dominant over recombination. In this paragraph this statement is confirmed via numerical analysis. Two simulations are performed: in one electrons are free to diffuse in the surrounding but do not recombine with ions, in the other one recombination is allowed but diffusion is not.

⁶Actually, Appendix B provides an explanation to this fact, based on the quasi-Maxwellian nature of the distribution function in the trail.



Figure 6.13: Number density of free electrons computed by LARSEN. Top: only diffusion. Bottom: only recombination. Meteoroid included for dimensions comparison.

Results are shown in Fig. 6.13 and clearly show that the prediction based on the Damköhler parameter was correct. In fact, in the simulated flight conditions, the flow is rarefied and this drastically reduces the number of molecular collisions that can lead to recombination reactions. This fact is especially true in the core of the trail, where the density is even lower as discussed in Section 6.2: the electrons concentration is seen to be particularly persistent in time.

Lagrangian correction of DSMC results

Finally, in this paragraph the Lagrangian solver will be applied to an improvement of the DSMC solution. Both diffusion and recombination effects have been introduced by the Lagrangian solver and results are shown in Fig. 6.14. Those results provide the sought map of free electrons in region (ii).



Figure 6.14: Number density of free electrons corrected by LARSEN.

In order to estimate the importance of the Lagrangian correction, that adds recombination to the initial DSMC field, the result is compared to an additional simulation where chemistry was switched off. The free electrons concentration at the exit is given in Fig. 6.15 and clearly shows that chemistry plays a significant role.⁷ This result justifies all the efforts undergone in the development of the Lagrangian solver, since a very big improvement with respect to DSMC is shown.

The effect of recombination reactions in this first part of the trail is seen to generate a big variation in the number density of free electrons, reaching values of 40% at the core of the trail. A parameter often used in the meteor modeling field is the *line density* of electrons, that can be obtained by integrating the (volume) number density over the cross sectional area:

$$n_{line}^{e} = \int_{S} n^{e} R \,\mathrm{d}R \,\mathrm{d}\theta = 2\pi \int_{0}^{\infty} n^{e} R \,\mathrm{d}R \tag{6.2}$$

where the axial symmetry was introduced. This parameter gives more importance to the electrons at the sides of the trail and less to the core, due to the cylindrical nature of the flow. By comparing this parameter for the two simulation, still big changes can be seen, the free electrons line density being inferior by the 28% if recombination reactions are taken into account.



Figure 6.15: Number density of free electrons at the exit of computational domain. Effect of chemical reactions.

Those results remark how important is to take into account both diffusion and recombination processes if the density of free electrons in the trail is sought. While diffusion is absolutely prevalent in those flight conditions, recombination still plays a very important role.

Is should also be recalled that the obtained results depend on the particular flight condition that is simulated. Different altitudes, velocities and meteoroid sizes would probably generate very different results, with recombination becoming more and more important at lower altitudes.

⁷This does not contradict the estimation done with the Damköhler parameter, that is only stating that the effect of diffusion is much bigger. In fact, while chemistry changes the value by around the 30%, diffusion reduces the number density by approximately two orders of magnitude.

From the performed simulation, the number density of free electrons is found to be high enough to generate a *total reflection* of incoming radio signals. In fact, as reviewed by Pellinen-Wannberg et al. in [33], radio devices operating in the UHF band can detect free electron number densities as low as 10^{16} m⁻³, while VHF devices such as the BRAMS Network [4] can go even below, up to 10^{14} m⁻³. An extended domain is thus to be taken into account and is the object of the next section.

6.4.2 Lagrangian computation of the far trail

The analysis of the free electrons performed in the previous section predicts that a big number of electrons is still present at the exit of region (ii), enough to generate a total reflection of incoming radio waves. In other words, the trail length effectively reflecting radio signals is longer than what was simulated in the previous section. In this paragraph, the Lagrangian solver is applied to a further extension of the computation, up to a distance of 2 km from the meteoroid.

As was discussed in Section 6.10, the flowfield quantities evolve along the trail, approaching freestream conditions. Region (iii) was in fact defined as the region of the trail where the velocity and density reached uniform freestream values. Thus, if a solution is obtained for region (ii) in terms of species concentration, this data could be used as initial value and the Lagrangian solver could be applied to the simple flow conditions of region (iii) determining the free electrons distribution in the remaining of the trail. This is what is done in this section.

Unfortunately, the simulation performed of region (ii) proved to be *insufficient* for the density to completely reach freestream values. This fact will be neglected in this work, the main goal being linking all the necessary steps and building a sound fluid dynamic methodology for studying meteor trails. Obtained results will thus be *approximated*, but still *more realistic* than the currently employed state of the art methods.

The computational domain for this extended simulation is a box of $2000 \text{ m} \times 4 \text{ m}$, shown in figure Fig. 6.16. Initial conditions are taken from the outlet of the previous simulation on region (ii) and specified at the inlet of this new computational domain. The specified initial conditions change from one streamline to the other in terms of electrons concentration and temperature, while the density and velocity are, as said, are taken equal to the freestream values (6.2).

In this simulation heat transfer is computed by the Lagrangian reactor in the radial direction, resulting in a progressive cooling of the trail until freestream conditions are reached. The result is shown in terms of free electrons concentration in Fig. 6.17. Only a portion of the computational domain is shown and was scaled to appreciate the diffusion phenomena.

This result is the final outcome of the current work.



Figure 6.16: Domain for the simulation of region (iii), with a sketch of the diffusing ionized region.



Figure 6.17: Number density of free electrons in logarithmic scale, as computed by the Lagrangian solver. Axis are scaled.

Analysis of the recombination process

The effect of recombination reactions can be understood by observing the total amount of ions and free electrons⁸ on a cross section at a given trail position. In fact, this quantity changes only due to chemical reactions, since diffusion simply redistributes radially the species. The number density of species (atoms or molecules per cubic meter) was thus cumulated on the cross section according to equation 6.2, giving the number of molecules per unit length along the trail.

Fig. 6.18 clearly shows how recombination takes place: first of all a part of free electrons recombines with the N_2^+ ions, determining the first part of electrons diminishing. A very small quantity of NO^+ can be spotted in the initial part of the trail, contributing to the free electrons balance only in very small quantity. The second species to start recombining is N^+ , and the third one -although this cannot be appreciated from the performed simulation- will probably be O^+ , as discussed in the following.

The explanation of this phenomena is conceptually simple: the ionization energy of N_2 is the highest, so that at low temperatures electrons easily recombine. The second recombination mechanism is seen to happen for N, whose ionization energy is smaller than N_2 but bigger than O. The ionization energies for those three species are reported

⁸Actually, those quantities are the same due to the ambipolar assumption employed in this project.

in table 6.5, from the NIST WebBook [34].

species	ionization energy $[eV]$
N_2^+	15.5
N^+	14.5
O^+	13.6

Table 6.5: Ionization energy for the main ions in the air gas mixture.



Figure 6.18: Line density of ions and electrons along the trail, up to 2 km from the meteoroid.

Such recombination path is obviously based on the chemical mechanism used in the simulation, that in this work was taken from [25]. However, although the qualitative behavior could have been guessed *a priori*, a quantitative prediction needs to couple the chemistry with diffusion effects due to the dependence of chemical rates on the local concentration of chemical species.

It is possible to predict on qualitative grounds what the behavior of the recombining trail would be at different altitudes: in fact, the simple problem of isothermal recombination admits a self-similar solution with respect to the the variable P^2t , so that at a given the altitude the recombination times can be qualitatively estimated. The reason for the similar behavior lies in the nature of recombination reactions, that arise due to three-body collisions and is treated in more detail in Appendix C.

Once a map of free electrons is obtained, it can be plugged into an electromagnetic solver able to quantitatively study the scattering process for radio waves and a received signal can be reconstructed. A series of calculations on meteoroids of different sizes can be performed following the same path that was developed in this work, and a database can be thus obtained for a quick interpretation of received radio signals.

Finally, modeling ablated species in the trail is also possible with the developed approach: what is needed are initial concentrations of species, together with the necessary thermodynamic and transport properties of ablated elements.

Chapter 7

Conclusions and future work

7.1 Conclusions

In this work, a methodology for studying free electrons in meteor trails was proposed. This methodology has its roots in fluid dynamics and fills a gap in the literature, where the fluid nature of the problem is brutally approximated or even neglected. During this work the importance of a careful flow modeling was highlighted, showing deviations of the results up to the 30% if a comprehensive treatment of *both* diffusion and recombination is not performed.

As defined in the beginning of this work, if an accurate description of the free electrons evolution in meteor trails is sought, some key points need to be considered:

- **Consideration 1)** Meteor trails are *fluid dynamics* entities and the current state of the art neglects this fact. Moreover, they are typically rarefied;
- **Consideration 2)** Trail simulations require detailed chemical mechanisms to be accounted for and current rarefied flow solvers cannot properly introduce them;¹
- **Consideration 3)** Trails are very extended in size and classical methods prove to be exceedingly computationally demanding.
- Those facts have been directly addressed in this work, obtaining a result for each of them:
- **Result 1)** Simulations of the flow around and past a meteoroid were performed and the trail was characterized from the fluid flow point of view, defining its three composing regions. Simulations were performed with the DSMC method, vastly used in the aerospace field and tailored to rarefied flows.
- **Result 2)** A Lagrangian reactor able to introduce detailed chemical models in previous baseline simulations was developed. The solver provided a correction of the performed DSMC simulations, introducing recombination reactions and thus providing a map of free electrons in the first part of the meteor trail (Fig. 7.1).

¹Recombination reactions in DSMC solvers are still an open issue.

Result 3) The Lagrangian nature of the developed solver makes it particularly lightweight: thanks to this property it was possible to simulate a very long trail, with an extension of 1 km.

The reactive fluid dynamics software here developed was based on a previous work of the author at VKI [29]. In this work the validity of the decoupling performed by this solver is discussed and seen to be valid for the tried testcases.

The current work focused on making this solver suitable for meteor trails analysis. In particular, this implied implementing processes of mass and energy diffusion. The developed solver was verified against simple testcases for both diffusion of mass end energy in 2D Cartesian and axisymmetric geometries. An additional *a posteriori* verification for the mass diffusion implementation was obtained by comparing the results with the meteor DSMC: results are close to each other and the diffusion process seems thus well captured by the Lagrangian reactor.



Figure 7.1: Simulation of free electrons in the near trail of a meteor.

From the performed trail computations, it was found that the ionized trail is very persistent at the flight conditions studied (entry velocity of 20 km/s and altitude of 70 km). In fact, for a meteoroid of 1 cm diameter the ionized portion of the trail was found to exceed a length of 1 km.

The map of electrons obtained in this project can be fed to an electromagnetic software and an estimation of the reflection of radio waves can be obtained. In this way, it's possible to create a database of meteor trails and received experimental signals can be used to estimate the size of incoming meteoroids.

The developed Lagrangian tool, named LARSEN, is able to obtain in a matter of minutes - on a laptop - a result that would otherwise require probably weeks of computation on modern supercomputers if the DSMC method would be used. All the gain is due to the parabolic nature that the equations assume when longitudinal diffusion is neglected, an approximation holding well in meteor trails.

7.2 Not only meteors: other applications

Although applied to the study of meteor trails, the Lagrangian reactor LARSEN was developed to be as general as possible. In the near future the code will be applied to a

number of different applications, a few of them are here provided as an example.

Blackout around the ExoMars capsule

The entry phase of the ExoMars capsule in the Mars atmosphere led to a period of interruption of radio communications due to the formation of a layer of ionized gas, reflecting away radio waves and thus shadowing the capsule antenna. This issue is a well known phenomena in the atmospheric entry of capsules and is known as *telecommunication blackout*. The Lagrangian reactor will be applied in the next future to this testcase, trying to reproduce experimental results.



Nonequilibrium population of xenon gas in hall-effect thrusters



Recently, very detailed models became available for the energy levels of xenon gas. Their interaction can be studied using a "state to state approach", where the energy levels are treated as pseudo-species and the exchange of energy as pseudo-chemical reactions.

The Lagrangian solver will be applied to the determination of the energy level excitation in the plume of a hall thruster starting from a simulation of a few levels only.

7.3 Future work

In this section, some future work directions are suggested for both the development of the Lagrangian solver LARSEN and for the modeling of meteor trails.

Further development of LARSEN

The developed solver is now able to treat chemical reactions as well as diffusion of mass and energy across streamlines. Further implementation could extend the power and range of applicability of the solver. In particular, suggested developments are:

- Implementation of multi-temperature models, starting by a two temperatures $T T_v$ approach. This would allow to take into account nonequilibrium flows as well.
- Implementation of collisional-radiative models and radiative processes (for example the radiative recombination process $N^+ + e^- \rightarrow N + h\nu$). This would allow for the description of nonequilibrium among energy levels and also provide additional recombination mechanisms to free electrons.
- Implementation of barotropic diffusion and Soret effect in the mass diffusion model.

- Implementation of the power of viscous forces in the energy equation, rightfully neglected in meteor trails but important in other types of flow.
- Verification of the implemented mass and energy diffusive fluxes for non-trivial testcases, using CFD and DSMC approaches.

Simulations of meteor trails

Regarding the modeling of the meteor phenomenon and in particular the simulation of free electrons in meteor trails, some suggestions for future work are:

- Repeating the performed simulations with more complex air chemical models.
- Adding ablated species into the trail and studying the effect of different meteoroid chemical composition on the trail shape.
- Applying an electromagnetic solver to the computed maps of free electrons to obtain the entity of the reflected signal. Raytracing programs could be used as an initial step, to assess whether the radio wave is able to penetrate the trail or is totally reflected, at a given free electrons density.
- Performing a series of simulations on meteoroids of different sizes and velocities to obtain a parametric study of how characteristic trail quantities (such as the length and maximum diameter of the ionized region) depend on the meteoroid dimension and flight conditions.

Appendix A

More on DSMC simulations

In this appendix are shown more details and results on the performed DSMC simulations of meteors.

A.1 Streamlines for the DSMC simulation

This annex briefly analyzes the streamlines behavior as found from the DSMC simulations performed in chapter 6. In section 6.2, the density was seen to follow a different behavior than the velocity and temperature fields. In fact, while the latter two monotonically approach freestream values along the trail, the density field is found to start increasing but soon it decreases again. The reason for this behavior was attributed to the vertical component of the velocity field: this annex supports this hypothesis showing the streamlines behavior in the trail.



Figure A.1: Streamlines near the meteoroid, reconstructed from DSMC solution.

Fig. A.1 shows the streamlines near the meteoroid, as reconstructed from the DSMC solution. As can be seen, right after the meteoroid some streamlines tend to fill the trail, thus causing an increase in the density. A scaled view of the streamlines allows for a better interpretation and is provided in Fig. A.2.

Fig. A.2 provides a more intuitive view of the flow behavior. Initially streamlines fill the trail, as previously said, and correspondingly the density along the trail increases



Figure A.2: Streamlines reconstructed from DSMC solution, scaled view in the x direction.

(section (A) in the figure). In the meanwhile, streamlines above cross the diffused bow shockwave and extend vertically (section (B) in the figure). This vertical movement has the effect of "pulling up" the streamlines in the trail (section (C) in the figure), thus generating a further decrease in the density along the axis.

This interpretation is coherent with the density plot along the axis, given in Fig. 6.9, where around the position x = 0.3 m the density stops raising and starts decreasing again. Eventually, as freestream conditions are reached, streamlines will close again to meet the initial configuration.

A.2 Simulations at different entry velocities

This appendix compares two DSMC simulations of a 1 cm meteoroid at an altitude of approximately 70 km. Two flight speeds are compared: 20 kms and 72 kms. Those simulations are approximately located at the boundaries of the entry velocities of meteoroids in the Earth's atmosphere, usually ranging from 12 to 72 km/s.

Fig. A.3 shows a comparison of the temperature fields around the body and in the first region of the trail. An increased temperature is seen for the higher velocity case, where the value is one order of magnitude higher. It's important to recall that at the considered rarefaction conditions, those temperatures are *geometrical temperatures*, as discussed in section 4.4, and are not indicative of the thermal agitation of the gas.

The number densities are compared in Fig. A.4. The simulation at higher velocity shows a much more well-defined trail: the contribution of mass diffusion with respect to advection is smaller in the higher velocity trail and the result is a much more extended region of low density in the shadow of the meteoroid.

$T_{max} = 1.56E + 06 K$	
T _{max} = 1.32E+05 K	
<u> </u>	0 Translational temperature [K] 1e+05

Figure A.3: Comparison of temperature fields. Top: 72 km/s. Bottom: 20 km/s.

$n_{max} = 1.74E + 24 m^{-3}$		
n _{max} = 1.77E+23 m ⁻³	2e+21	4e+21
	0 Number density [m ⁻³]	5e+21

Figure A.4: Comparison of number density fields. Top: 72 km/s. Bottom: 20 km/s.

A.3 Effect of chemistry on flowfield quantities

In chapter 6, DSMC simulations were discussed and features of the flowfield were analyzed. The question of whether such features would drastically change if electrons recombination would be modeled arose: this question is partially answered in this appendix. An additional simulation was thus performed switching off totally chemical reactions and results were compared with the reactive simulations discussed in the main work. This allows to test how strong is the link among chemistry and flow quantities.

The freestream air mixture is composed by molecular oxygen and nitrogen only, in the same conditions as the testcase of chapter 6.



Figure A.5: DSMC computational domain for comparison among chemical models

Fig. A.5 shows the computational domain, that extends up to 0.775 m, or 77.5 meteoroid diameters. Flow quantities have been extracted along the trail axis and are shown in Fig. A.6 and A.7.

Some observations can be made:

- the velocity field is almost identical for the two simulations
- the density field as computed with the two models initially differs, but after 0.3 m (30 diameters) results are again the same



Figure A.6: Comparison of velocity and density for the two chemical models.



Figure A.7: Comparison of translational, rotational and vibrational temperatures.

• the preficted translational and rotational temperatures are very close to each other for the two models. The vibrational temperature is the one that changes most.

A departure of results in terms of temperature is expected since chemical reactions release or adsorb energy. However, the difference is seen to be relatively small in the long-run. The models departure is bigger for the vibrational energy, which is notoriously linked to chemical reactions.

To sum up, the main features of the flowfield - the velocity and density fields - are seen to vary little even with a complete variation of the chemical model. This provides a good reson for trusting the employed Lagrangian approach, where an initial simulation is recomputed and deeply refined by the Lagrangian reactor. In fact, one may argue that baseline simulations with different chemical models might lead to very different results when the Lagrangian refinement is applied: those results suggest that this is not necessarily the case since even an extreme perturbation to the chemical model (chemistry totally switched off) is shown to generate relatively small deviations.

Of course, the preceding statements are limited to the present case-study.

Appendix B Statistical analysis of the trail

As discussed in chapter 4, the DSMC method is a stocastic way of solving the Boltzmann equation. As such, the information carried in the DSMC solution is not limited to the temperature, velocity and density fields, but is much richer: the DSMC method provides an estimation of the velocity distribution function, carrying information on the microscopic state of the gas in each point of the domain. In fact, temperature, velocity and density are just *mathematical moments* of the velocity distribution function.

In this section, the velocity distribution of particles is extracted from the solution and analyzed. Three points at different trail locations are here compared, their position being schematized in Fig. B.1.



Figure B.1: Sampled points for distribution function analysis.

From a practical point of view, the DSMC software was asked to output on a file the properties of the particles located in a certain grid cell. Particle properties are collected for a big number of timesteps and the distribution of velocities is obtained. Although conceptually simple, obtaining a smooth distribution from the DSMC sampling requires collecting a huge number of particles and this implies heavily increasing the number of timesteps and thus very long simulation times. For practical reasons, results shown here are thus obtained for a *non-reacting* mixture, since switching off the computation of chemical reactions considerably speeds-up the simulation. Results are believed to be indicative for the reacting simulations as well, at least from a qualitative point of view.

The raw data was used to compute a distribution of velocities for the particle in the sampled cells and the result is shown in Fig. B.2 for the three trail locations. The plotted

curves represent the number of particle with a certain velocity c_x or c_y respectively in the x and y direction. Those curves are thus closely related to the marginal velocity distribution functions $f(c_x)$ and $f(c_y)$, the difference being merely a matter of scaling.



Figure B.2: Velocity distribution of particles at three locations along the trail.

It can be observed that the velocity distribution in the radial direction shows two peaks. This feature is due to the rarefied nature of the considered flow and can be explained by the fact that atoms or molecules in a rarefied gas travel long distances before colliding with another particle. Some molecules located above the axis, are then able to reach it with a finite velocity and cross it, as shown in Fig. B.3. The same happens for molecules located *below* the axis, so that if the average is computed, the velocity is found to be parallel to the symmetry axis and the basic principle that "streamlines don't cross each others" is of course respected. The two peaks are seen to quickly merge into one and the shape of the velocity distribution starts resembling a Maxwellian already

	Point (A)	Point (B)	Point (C)
T [K]	42374	24749	17151
T_x [K]	45115	29382	20077
T_y [K]	41274	22269	15601
T_z [K]	40694	22596	15776

Table B.1: DSMC simulation: anistotropy of temperature along the trail axis.

after a few diameters in the trail.



Figure B.3: Sketch for streamlines approaching the symmetry axis.

From this information over the particle velocities it's possible to obtain the distribution function and temperatures can be computed in the two velocity directions. As explained in chapter 4, although the temperature is classically depicted as a scalar field, *anisotropy* may be observed at the molecular scale. In particular, the temperature was computed from the distribution functions in the three axis directions x, y and z and are found to be slightly anisotropic. The values are compared in table B.1.

As the trail develops, those values collapse on each other as effect of the thermalization. Two observations can be made:

- the radial temperatures T_y and T_z are very close to eachother, in fact those directions are totally equivalent, both being radial and perpendicular to the trail axis
- the longitudinal temperature T_x is seen to be higher than the radial ones and the temperature T accordingly results having a value which is intermediate among them.

The reader is referred to chapter 4 for more explaination on those effects, usually neglected in classical fluid dynamics.

The results obtained in this section are qualitative, but of big impact: they constitute the basis for section 6.4 - the application of the developed Lagrangian solver. The fact that the velocity distributions quickly approach a Maxwellian and the temperature becomes isotropic allows us to use models that are characteristic of the continuum. In particular, diffusion models for mass and energy implemented in the LARSEN solver are inherently based on the continuum assumption. Chemical reaction rates are also based on continuum assumption, in that the Arrhenius law is formulated in the assumption of
Mawellian (gaussian) distribution. Those results basically legitimate the application of continuum methods in the analysis of the trail, which is the goal of section 6.4.

Appendix C

Similarity variable in isothermal recombination

In this appendix, the simple case of isothermal recombination is addressed and a similarity variable is identified. This problem somehow mimics the behavior of free electrons in the last part of a meteor trail, where the temperature and pressure are uniform and equal to the free stream conditions, but a number of electrons still await for recombination to occurr.

A sample reaction will be analyzed, but results hold in general for *three-body collisions*. The chosen reaction is three body recombination of an electron to an ion M^+ :

$$M^+ + 2e^- \to M + e^- \tag{C.1}$$

Charge neutrality imposes that $[M^+] = [e^-]$, where the square brackets denote the molar concentration $[\text{mol/m}^3]$. Using the law of mass action, the concentration of free electrons in time is described by:

$$\frac{d[e^{-}]}{dt} = -k \ [M^{+}][e^{-}]^{2}$$
(C.2)

where k is the recombination rate coefficient. Exploiting the charge neutrality condition and manipulating the equation:

$$\frac{1}{[e^-]^3} \,\mathrm{d}[e^-] = -k \,\mathrm{d}t \tag{C.3}$$

The solution in time is easily found to be:

$$[e^{-}](t) = \left[\frac{1}{[e^{-}]_{0}} + \frac{k}{2}(t - t_{0})\right]^{-1/2}$$
(C.4)

where the subscript 0 refers to the initial condition.

If the definition of the molar concentration is then introduced, $[e^-] = n_e / \mathcal{N}_A$, the solution can be written as:

$$\frac{n^{e}(t)}{n_{0}^{e}} = \frac{1}{\sqrt{1 + \frac{k}{2} \left(\frac{n_{0}^{e}}{\mathcal{N}_{A}}\right)^{2} (t - t_{0})}}$$
(C.5)

And finally, introducing the perfect gas equation $n = P/k_BT$ and the definition of the molar fraction $X_e = n_e/n$, gives:

$$\frac{n^e(t)}{n_0^e} = f(P^2 t) = \frac{1}{\sqrt{1 + \frac{1}{2k_B T^2} \left(\frac{X_0^e}{\mathcal{N}_A}\right)^2 P^2 t}}$$
(C.6)

The solution is thus seen to only depend on the similarity variable $\xi = P^2 t$. Threebody recombination due to collision with molecules other than electrons as a third body provide the same dependence.

A number of numerical simulations were performed at various altitudes to compute the recombination of free electrons in an air mixture, starting from a totally ionized case. Fig. C.1 and C.2 show the values for temperature and pressure at various altitudes, according to the 1976 standard atmosphere. Values were extracted for altitudes from 20 to 80 km.



Figure C.1: Temperature in the 1976 standard atmosphere.



Figure C.2: Pressure in the 1976 standard atmosphere - linear and logarithmic scales.

The results of the recombination simulations are shown in Fig. C.3, where the time was plotted logarithmically for ease of representation.

Since at every altitude the number density is different, the value is adimensionalized by the initial number density of free electrons. The result is shown in Fig. C.4.

If finally the scaling suggested is applied to the horizontal axis, the curves at the various altitudes are seen to collapse on one only curve, as shown in Fig. C.5.

Finally, the process is valid for all the three body recombinations, even among nonionized species, so that the whole mixture is seen to follow the scaling.



Figure C.3: Recombination process at different altitudes.



Figure C.4: Recombination process at different altitudes - adimensionalized.



Figure C.5: Recombination process in the similarity variable.



Figure C.6: Recombination process in the similarity variable - all the species.

From the similarity solutions, a characteristic time can be extracted (based for example on a recombination equal to 99%) and a crude estimation for the lifetime of free electrons in the meteor trail can be found.

The effect of the freestream temperature can be studied as well, and is shown in Fig. C.7.



Figure C.7: Recombination process in the similarity variable at various temperatures.

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