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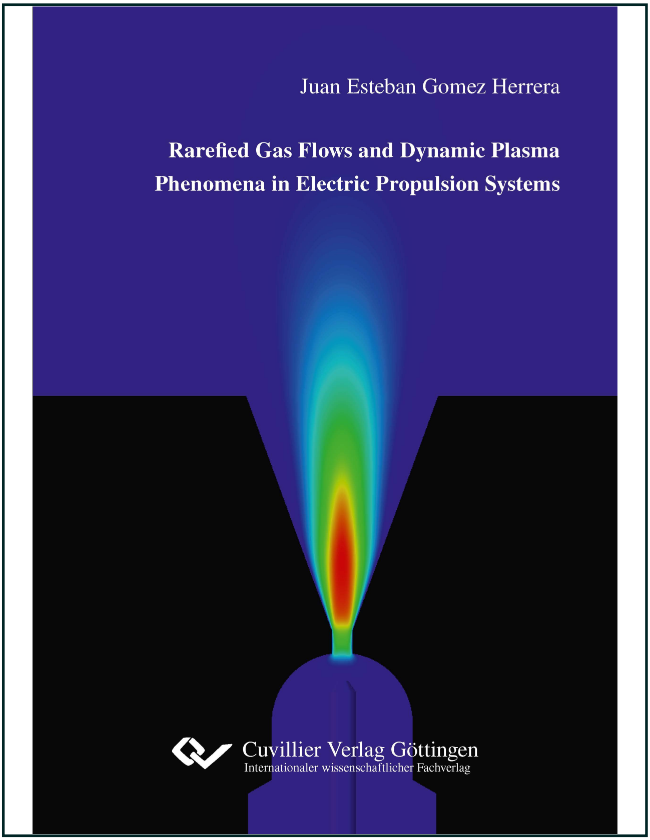
Rarefied Gas Flows and Dynamic Plasma Phenomena in Electric Propulsion Systems



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Chapter 1

Introduction

For over a decade, the group Thermofluid Dynamics at the Center of Applied Space Technology and Microgravity (ZARM) has performed both experimental and numerical work in a variety of research fields including turbulent and convective flows, electrodynamics and magneto-fluid dynamics. One of the technical applications offering the greatest potential in terms of research scope, relevance and applicability is the field of propulsion systems for spacecraft. Besides the undeniable importance from an engineering standpoint, the study of thermodynamic phenomena in cold-gas and electric propulsion devices is closely related to complex scientific research topics like rarefied gas conditions, transonic and supersonic flows, magnetohydrodynamics and plasma dynamics. In these particular fields, several experimental studies using diverse thermo-electric arcjet thruster setups as well as numerical investigations employing custom models and numerical approaches have been performed at ZARM. The present work takes advantage of an existing experimental setup for a miniaturised arcjet thruster referred to as *Ionised Noble Gas Accelerator* INGA III in an attempt to gain a deeper understanding of transonic micronozzle flows in rarefied gas conditions, as well as to develop and validate a numerical model able to describe plasma-dynamic phenomena inside electric propulsion systems for spacecraft applications.

1.1 Motivation

In recent years, several new trends regarding fundamental characteristics of orbital spacecraft have originated inside the space industry. One of them is the increased interest in miniaturized satellites (e.g., CubeSats) with the ability to perform spacecraft formation flying. As a result, the development of small propulsion systems based on Micro-Electro-Mechanical-Systems (MEMS) and able to provide small and precise thrust and impulse levels has become an important research topic. The required low propellant mass flow rates and the small characteristic lengths of such devices lead to gas rarefaction effects in the micronozzles of the thrusters becoming dominant factors affecting both general behaviour and performance of the propulsion systems. For this reason, the study of the effects of the associated high Knudsen numbers in micronozzle transonic flows as well as their numerical modelling constitute research fields of growing importance and applicability.

In addition to the increased interest in miniaturized spacecraft as a viable option to meet orbital satellite requirements, recent years have also seen a considerable rise in the use of electric propulsion systems for orbit and attitude control of standard-sized satellites, complementing classic chemical and cold-gas devices. Electric propulsion devices enable the generation of very low and precise thrust values, a feature which at the same time is key for the attitude control of miniaturized satellites. In addition, the much higher specific impulse values I_{sp} achievable with electric devices highlight their inherent superior efficiency compared to cold-gas and chemical systems. Because of the high complexity of the plasma dynamic phenomena taking place inside electric propulsion systems and the usually very high computational requirements associated with their numerical modelling, electric propulsion systems for space applications are usually designed based on empirical models and experimental data. However, considering the always increasing computational power as well as the potential in terms of technical optimisation and development costs reduction, the exploration of new approaches for the modelling of such systems becomes more attractive every day. From a scientific standpoint, research work in this field offers plenty of opportunities to improve the understanding of complex dynamic plasma phenomena, energy exchange and transport mechanisms, not only inside electric propulsion devices, but also in other plasma systems.

1.2 Basic setup

In the present work, both experimental and numerical tools are employed extensively. The INGA III thruster setup at ZARM shown in Fig. 1.1 is used for the experimental study of transonic cold-gas flows under rarefied gas conditions. The main component of the setup is the Laval nozzle shown schematically in Fig. 1.2 which in turn, is installed inside a spherical vacuum chamber with a total volume of approximately 10 litre. In cold-gas operation mode, the thruster is capable of accelerating the noble gases xenon, krypton, argon and neon to supersonic conditions, transforming this way the thermal energy of the compressed propellant gas into kinetic energy. Vacuum conditions in the spherical chamber are achieved using a commercial rotary vane pump. The setup includes, among others, mass flow rate and pressure measurement devices allowing the determination of the gas pressure drop through the Laval nozzle as a function of the propellant type and its mass flow rate. In the frame of this work, the obtained results are compared with numerically obtained data in order to examine in detail the effects of rarefied gas conditions on the system as well as to identify potential efficiency improvement strategies.

Figure 1.1: INGA III experimental setup with Laval nozzle fixed on the top lid of the spherical vacuum chamber.

Cold-gas numerical simulations are performed using standard continuum-based and kinetic Direct Simulation Monte Carlo solvers included in the software package *OpenFOAM*®. Furthermore, a Particle-in-Cell with Monte-Carlo collisions numerical model is developed and validated in the present work. The model, which includes key elements for the accurate modelling of plasma-dynamic behaviour inside electric propulsion systems, is based on the solver *dsmcFoam* of *OpenFOAM*®. In this thesis, the developed solver is shown to reproduce basic plasma dynamic phenomena as expected inside electric propulsion devices like the INGA III thruster. The numerical simulations with high computational requirements for both the cold-gas operation as well as for the validation of the developed custom plasma solver were performed in the ZARM computational cluster as well as in the super computer of the North-German Supercomputing Alliance (*Norddeutscher Verbund zur Förderung des Hoch- und Höchstleistungsrechnens - HLRN*).

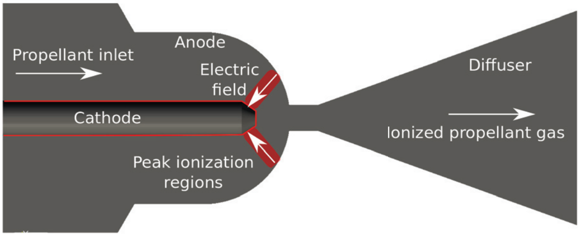

Figure 1.2: Schematic representation of the Laval nozzle in the INGA III setup and basic elements of the hot-gas arcjet operation mode.

1.3 Goals and thesis outline

The main goals of the present thesis are the investigation of gas rarefaction effects in transonic micronozzles flows and their impact on system behaviour and performance as well as the development of a numerical kinetic modelling concept able to accurately describe dynamic plasma phenomena inside electric propulsion devices with acceptable computational requirements. The detailed structure of this work is described in the following.

In Chapter 2, theoretical principles linked to the performed studies are outlined. The focus of the chapter lies on the definition of the different flow regimes as a function of the Knudsen number. Based on this, conservation equations for the description of flows in the continuum regime are developed and discussed. Furthermore, the working principle of the Laval nozzle, a common element of chemical, cold-gas and thermoelectric arcjet thrusters, is described. In order to establish a theoretical basis for the development of a kinetic plasma model, fundamental concepts of the plasma state and the kinetic description of gases are introduced in the final sections of this chapter.

Chapter 3 is dedicated to the computational methods employed for the numerical studies performed in the present work. The chapter introduces typical spatial and temporal discretization schemes for conservation equations valid in the continuum regime, as well as commonly used solution algorithms. In addition, the Direct Simulation Monte Carlo method (DSMC), widely employed for flows under rarefied conditions, is outlined. The chapter ends with a description of the Particle-In-Cell (PIC) algorithm, which combined with the DSMC method, constitutes the basis for the numerical plasma model developed in the frame of this thesis.

The experimental and numerical study of cold-gas transonic flows across multiple flow regimes is presented in Chapter 4. Here, gas rarefaction conditions in transonic micro-nozzle flows and their impact on system behaviour and performance are examined taking advantage of the INGA III experimental setup. Furthermore, comparisons between different numerical approaches in the slip-flow and transition regimes are performed. Finally, the chapter introduces a new gas-independent correcting relation as a function of the Knudsen number and applicable to continuum-based Navier-Stokes results under rarefied gas conditions.

Chapter 5 is dedicated to the development of a global numerical modelling concept for the simulation of plasma phenomena inside electric propulsion systems like the INGA III arcjet thruster in hot-gas operation mode. The hybrid modelling concept is based on the coupling of a kinetic submodel for plasma phenomena with a fluid submodel for ohmic gas heating and neutral gas handling. The kinetic plasma submodel is fully developed in the frame of this thesis based on the Particle-In-Cell (PIC) algorithm and Monte Carlo collisional schemes. The obtained kinetic solver, referred to as *dsmcPlasmaFoam*, includes short-range Coulomb collisions between charge carriers, electron-neutral interactions linked to gas ionisation as well as dynamic test particle weighting for computational optimisation.

The main components of the developed solver *dsmcPlasmaFoam* are analysed and validated in Chapter 6. They include the Maxwell solver for the determination of the electric field from a kinetic particle distribution, the Lorentz solver describing the charge carriers motion in an electric field as well as the weighting steps for the computation of the particle density from the particle distribution and the electric force acting on the charge carriers. Furthermore, validation cases for the short-range Coulomb interactions model as well as for the implemented electron-neutral collisional approach are presented. The results discussed in this chapter confirm the solver *dsmcPlasmaFoam* as a powerful, flexible and accurate modelling tool covering a wide range of typical plasma phenomena. The developed solver is expected to serve as one of two main submodels in the envisioned hybrid PIC-MCC-FVM plasma model currently in development at the Center of Applied Space Technology and Microgravity (ZARM).

Chapter 2

Theoretical Principles

In this chapter, the theoretical principles and main governing equations required for the modelling of the cold-gas and hot-gas operating modes of an electric propulsion system are presented. The chapter begins with a brief introduction of the Lagrangian and Eulerian specification of the flow field followed by the mass and momentum conservation equations as well as the ideal gas law. The final sections of the chapter are dedicated to the Laval nozzle, fundamentals of plasma phenomena and the kinetic theory of gases.

2.1 Knudsen number and flow regimes

Let λ represent the mean free path in a fluid, i.e., the mean distance covered by a particle or molecule before a collision with a second particle takes place. In this case, the dimensionless Knudsen number Kn is defined as the ratio between the mean free path λ and a characteristic geometrical length l as follows:

$$Kn = \frac{\lambda}{l} \tag{2.1}$$

For low values of Kn, the mean distance covered by a particle before a collision with a second particle takes place is small in comparison with the characteristic length of the system. This is the case for gases with relatively high densities and a regular molecular distribution or for problems with large geometrical scales. On the other hand, high values of Kn are present when the particle density in the system is low or when the problem involves small geometrical scales. In this case, the probability of a particle interacting with a domain boundary before it collides with a second particle is relatively high. Based on the above, the Knudsen number Kn enables the definition of the flow regimes shown in Table 2.1.

Continuum regime	0	$< Kn <$	10^{-2}
Slip flow	10^{-2}	$< Kn <$	10^{-1}
Transition regime	10^{-1}	$< Kn <$	10
Free molecular flow	10	$< Kn <$	∞

Table 2.1: Flow regimes [Hän04].

In the **continuum regime** (low Knudsen numbers), the mean free path of the gas particles is much smaller than the characteristic length of the problem and the fluid can be mathematically handled as a continuum. Macroscopic quantities are obtained through averaging of the corresponding molecular quantities in a volume of the order l^{*3}. Here, l^* represents a geometrical length between the mean free path of the fluid λ and the characteristic length l of the studied system ($\lambda < l^* < l$) and can be imagined as the transition scale between the molecular and the continuum length scales (cp. [Pop00]). The control volume can therefore be divided into mathematical infinitesimal volumes, allowing the description of macroscopic quantities and their spatial and temporal changes through sets of partial differential equations. The most important set of partial differential equations for the flow description in the continuum regime are the Navier-Stokes-Equations [Hän04]. They are introduced in Section 2.4 of this work.

Relatively high Knudsen numbers in the range $10^{-2} < Kn < 10$ correspond to the **slip flow** and **transition regimes**. Here, the results from the Navier-Stokes-Equations with classic no-slip boundary conditions deviate from experimentally obtained data and a local thermodynamic non-equilibrium region known as the Knudsen layer becomes important. In this layer, the diffusive nature of the collisions between gas atoms and walls leads to a loss of momentum in the flow direction. This effect is, however, weaker than for gases in the continuum regime. Classic approaches for the description of flows with these characteristics are based on the formulation of modified boundary conditions for the near-wall velocity profile. These include first-order and second or higher-order slip boundary conditions.

The extreme case of high Knudsen numbers corresponds to the **free molecular flow**. Because of the very high values of λ and small geometrical dimensions, the particles rarely collide with each other before interacting with the domain boundaries. As a consequence, a thermodynamic equilibrium cannot be reached in the gas and the macroscopic state of the medium depends strongly on the state of individual particles. In this case, differential equations become inadequate for the flow description. Instead, flows in this regime can be accurately described through the kinetic theory of gases and the Boltzmann equation, which is, in theory, valid for all flow regimes. Since mathematical solutions of the Boltzmann equation are complex, numerical methods such as the Direct Simulation Monte Carlo method (s. [Bir94]) are usually employed [Hän04]. In Sections 2.2 to 2.6 of this work, the theoretical principles and main equations for the description of flows in the continuum regime at low Knudsen numbers are introduced. Furthermore, Section 2.9 is dedicated to the kinetic theory of gases, commonly employed for the description of flows at high Knudsen numbers.

2.2 Lagrangian and Eulerian specification of the flow field

Let us consider a flow in the continuum regime. The *Eulerian* specification of the flow field corresponds to the case in which specific locations in space are observed as the flow passes by. The *Eulerian* density and velocity fields can be defined here as $\rho(x,t)$ and $u(x,t)$ respectively, where x denotes an specific location in space. In contrast, in the *Lagrangian* specification of the flow field, the observer moves with the local velocity of the fluid. Let Y be the position of a specific fluid particle at a reference time t_0. As shown in Fig. 2.1, the position of the particle at any different time can therefore be defined as $X^+(t,Y)$ (cp. [Pop00]).

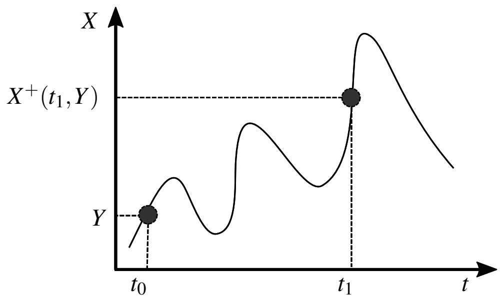

Figure 2.1: Trajectory $X^+(t,Y)$ of a fluid particle. Y represents the particle's position at the reference time t_0 (cp. [Pop00]).

Thus, any given fluid particle can be defined by an equation for the particle's position Y at the reference time t_0,

$$X^+(t_0, Y) = Y \tag{2.2}$$

and an equation for its velocity,

$$\frac{\partial}{\partial t} X^+(t, Y) = u(X^+(t, Y), t) \tag{2.3}$$

or alternatively,

$$u^+(t, Y) = u(X^+(t, Y), t) \tag{2.4}$$

Equation 2.4 establishes the relation between the *Lagrangian* velocity u^+ and the *Eulerian* velocity u and indicates that the particle's velocity u^+ is the same as the local flow velocity u [Pop00]. Furthermore, a similar expression can be formulated for the density:

$$\rho^+(t, Y) = \rho(X^+(t, Y), t) \tag{2.5}$$

Since the Lagrangian fields are defined by the particle's position Y at the reference time t_0, Y is known as the *Lagrangian* or material coordinate [Pop00]. The partial derivative of the *Lagrangian* density represents the time-dependent change of the density for a constant value of Y, i.e., following a specific fluid particle:

$$\begin{aligned}
\frac{\partial}{\partial t}\rho^+(t, Y) &= \frac{\partial}{\partial t}\rho(X^+(t, Y), t) \\
&= \left(\frac{\partial}{\partial t}\rho(x, t)\right)_{x=X^+(t,Y)} + \frac{\partial}{\partial t}X_i^+(t, Y)\left(\frac{\partial}{\partial x_i}\rho(x, t)\right)_{x=X^+(t,Y)} \\
&= \left(\frac{\partial}{\partial t}\rho(x, t) + u_i(x, t)\frac{\partial}{\partial x_i}\rho(x, t)\right)_{x=X^+(t,Y)} \\
\frac{\partial}{\partial t}\rho^+(t, Y) &= \left(\frac{D}{Dt}\rho(x, t)\right)_{x=X^+(t,Y)}
\end{aligned} \tag{2.6}$$

where,

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i} = \frac{\partial}{\partial t} + u \cdot \nabla \tag{2.7}$$

represents the *material* or *substantial* derivative. The rate of change of velocity following a fluid particle (i.e., its acceleration) can be formulated in a similar way:

$$\frac{\partial}{\partial t} u^+(t, Y) = \left(\frac{D}{Dt} u(x, t)\right)_{x=X^+(t,Y)} \tag{2.8}$$

Therefore, the rate of change of flow fields following a fluid particle is described by both the partial derivative of the *Lagrangian* fields and the material derivative of the *Eulerian* fields (cp. [Pop00]).