Ar(4s) AND Ar(4p) EXCITED STATES IN AN ARC-JET USED FOR PLANETARY RE-ENTRY PLASMA SIMULATIONS

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ABSTRACT

Arc-jet is a performant and convenient tool for the simulation of planetary re-entry plasmas. Plasma properties of an arc-jet running with argon at low pressure and at lower power are calculated by two fluid Navier-Stokes codes. In the chemical processes, the level Ar(4s) and Ar(4p) are introduced.

INTRODUCTION

In our days, the space missions selected by the different agencies for the exploration of the planets of the Solar system, notably Mars, Venus and Saturn, are numerous. In many case, they present a hypersonic flight through a particular planetary atmosphere for a trajectory chosen for its aero-breaking or aero-capture properties before landing. These trajectories induce many complex phenomena due to the presence of a strong ahead shock wave, as molecule dissociation in the ambient gas, ionisation and radiation phenomena. These phenomena are related to a context of non equilibrium conditions (chemical and ionisation in non-equilibrium situation, non mawxellian electron distribution, non equilibrium between the kinetic, electronic, vibrational and rotational temperatures T,Te,Tvj,Trj, non Boltzmanian equilibrium between the populations of the different states). All these phenomena contribute to an energy transfert to the surface of the spacecraft. a precise knowledge of this energy is necessary to define and optimize the thermal protection system (TPS) of the spacecraft. The objective is a minimization of the weight of the TPS in order to decrease the cost of the mission maintaining a sufficient quality of security for the required restricting trajectories.

Today, it is still necessary to increase the knowledge of the re-entry phenomena and this is done by large research programs from the space agencies. These programs resort to theorical studies as well as numerical modeling or experimental measurements.

Different ground test facilities have been used to simulate the plasma conditions appearing around a spacecraft during its hypersonic entry in a planetary atmosphere: shock tubes, microwave plasma sources, inductively coupled torch (ICP) and arc-jets. Each plasma source exhibits specific advantages and disadvantages. The strength of Arc-jets lies inits capability to sustain a low pressure large size - around a meter - plasma flow during a long time – a few hours and with electron properties similar to the flight spacecraft conditions. However, the energy exchange differs from a shock wave (arc–gas exchange) and the Mach number is generally low and limited to a value around 4-5. However, arc-jet is currently considered as one of the most powerful tools for the study of re-entry plasmas.

For an arc-jet running at reduced pressure, two fluid models has been developed. The first one at the IEPE Institute of the University of Poznan using Navier-Stokes equations and a finite-difference scheme; a second one at the ICARE Institute at Orléans, using also a fluid description but with a finite volume model. These two plasma descriptions take into account arc-coupling effects, dissipative effects (gas viscosity, diffusion of the species, heat transfert, electron mobility), and ionisation processes. The first one introduces a thermal non equilibrium (*Te, T*) and is today limited to a description of an argon plasma flow. The second one introduces a thermal equilibrium ($T = Te$) but can be used for different gas compositions as *Ar*, N_2, N_2-O_2 (Earth), N_2-CH_4 (Titan), CO_2-N_2 (Mars). In these two descriptions, one introduces atoms and molecules (neutral species and ions), and electrons. A local electron neutrality condition between all the charged species is assumed because potential sheath near the surfaces are not introduced and the local scale of description is greater than the Debye length.

The different species are not only in their ground states, but also many excited level for neutral and ionized species are present in the plasma. The analysis of the population of the different excited species reveals a great interest for several domains.

Excited levels of a neutral species atom or molecule can play an important role for the ionisation process. Calculation of the different level populations is necessary to evaluate the emission spectra.

A few molecular levels can be used to estimate a “pseudo” vibrational temperature, generally obtained by the ground state and the first level (State to State - StoS- approach).

For each case, the level of coupling between the microscopic and the macroscopic descriptions has to be examined. In order to tackle this problem, a first study has been carried out with argon as gas for D.C. low pressure arc-jet.

From the Navier-Stokes model available in IEPE (code Papyrus), the plasma flow parameters inside an arc-jet are presented (electron density, electron temperature, pressure and heavy particle temperature along the arc-jet axis) and the electron density is compared to its calculation in equilibrium condition. Morever, from the plasma density and from the neutral concentration, the populations of Ar(4s) and Ar(4p) are calculated using the set of processes (electron collisions and radiative de-excitations). These two populations are calculated on different points along the arc-jet axis and for different arc intensities. From these results, the main processes involving these two states are determined.

From the Navier-Stoke model developed in ICARE, the plasma flow parameters inside the same arc-jet are presented but with a different approach than this used by IEPE at Poznan. The two excited states Ar(4s) and Ar(4p) as considered are pseudo-species and directly introduced in the chemical kinetic model by means of forward and backward rate of coefficients of specific excitation and ionisation reactions.

For these two models, the production rates (essentially electron collision excitation) and the probabilities of de-excitation have been evaluated by the laboratory LPGP using a big number of theorical codes ans also experimental data.

1. ARC-JET PLASMA SOURCE

The studied arc-jet is an axisymmetric D.C plasma source running at reduced pressure (Fig.1). A convergent-divergent nozzle made of copper operates as anode and the cathode is a small flat disk inserted near a cylindrical anode throat made of W, WTh or Zr. The throat is 4mm in length and 5mm in length. The conical divergent is 30° in half angle and 55mm in length. The arc is sustained between the cathode and the anode, each electrode having a separated water cooling circuit. The minimum of distance between anode and cathode is depending of the nature of the gas, generally around *1mm*. The discharge current is controlled by the arc power supply.

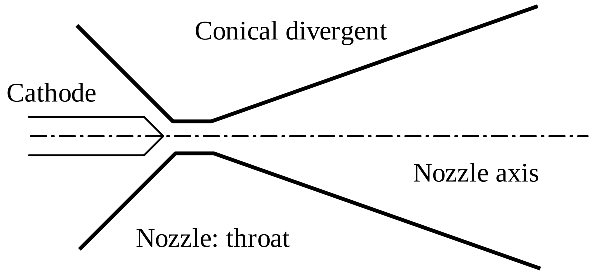


Fig.1 : Schematic view of the arc-jet

The plasma flow delivered by this arc-jet is assumed to be axisymmetric and stationary. At the exit of the nozzle, the flow is supersonic with a Mach number around 5.

2. PROPERTIES OF THE TWO Ar(4s) AND Ar(4p) LEVELS AND ATOMIC DATA EVALUATION

The 4s and 4p Ar I levels are between the most extensively studied rare gas levels, due to their intrinsic physical properties and because they generate spectral lines frequently present in various applications, both in the visible (4*s*-4*p*) and in the UV region (4*s*-3*p*). Of the four 4*s* levels (two with j_c= 1/2 and two with j_c= 3/2 in jK coupling description) two are transitory and two metastable, the transitions of the latter to the ground level (GL) being forbidden and difficult to observe in experimental plasmas. This fact contributes to an increased population of these levels in comparison with most excited states, to the point that their population cannot be negligible in comparison with the population of the GL. The ionization cross sections of the excited states being considerably higher than the one of the GL, the metastable 4*s* levels, even less populated than the GL, may significantly contribute to the overall plasma ionization.

The ten 4*p* Ar I lines (four with j_c= 1/2 and six with j_c= 3/2) cannot directly decay to the 3*p* ground level, a fact that contributes to somewhat increase their population, although all of them can easily decay to the lower situated 4*s* lines giving sixteen jK allowed transitions (Katsonis and Drawin, JQSRT **23** 1 1980). These constitute the well known stronger Ar red lines around 800 nm (followed in intensity by the blue lines coming from the 4*s* – 5*p* transitions) which significantly contribute to the 4*s* levels population. Seven among them lead to the two metastable 4*s* levels. Note that among the lower 4*p* levels, $2p_{10}$, $2p_9$, $2p_6$, the first and the last ones decay almost an order of magnitude easier to the metastable $1s_5$ than to the transitory $1s_4$, and the $2p_9$ decays practically only to the metastable $1s_5$. This fact confers a quasi-metastable character to these three levels.

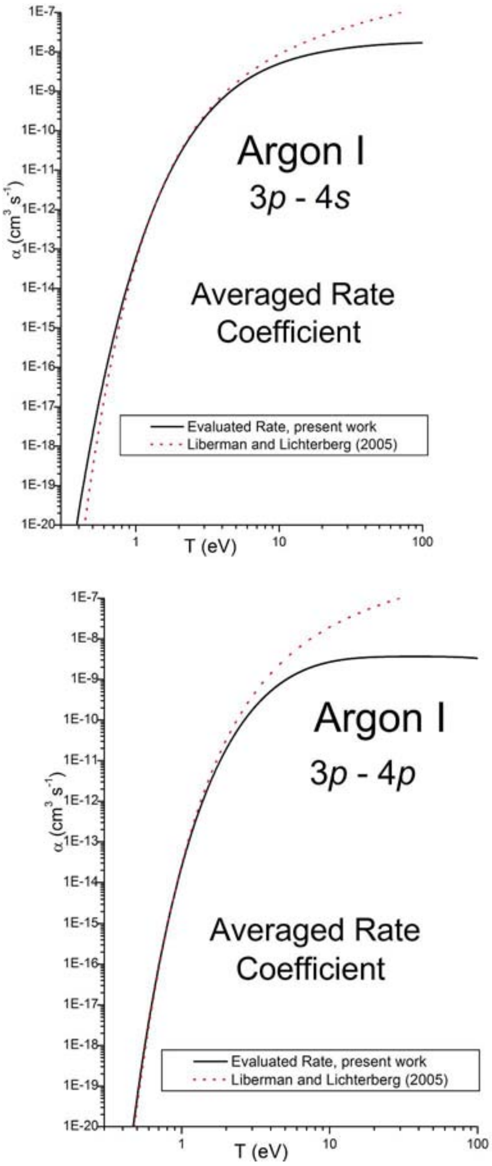
It becomes evident that if we seek a better consideration of the important atomic processes present in reentrance studies, we have to include in the models at least a collective representation of the four 4s and ten 4p levels, situated between the neutral Ar I GL and the ion Ar II GL. Here, the mean values of the atomic processes concerning the simplified 'four levels' atomic model (consisting of the Ar I GL, its continuum represented by the average of the two Ar II GL and the two global excited 4*s* and 4*p* levels) have been calculated from the data corresponding to the 14 individual lines and the two Ar II GL. Interestingly, in the often used LS coupling description, there is a strong mixing of the transitory 4s levels 3P1 ([3/2]1) and 1P1 ([1/2]1) ($1s_4$ and $1s'_2$ correspondingly in the Paschen notation) and of the 4p 3D1 ([3/2]1, $2p_7$), 1P1 ([1/2]1, $2p'_4$) and 3P0 ([1/2]0, $2p_5$), 1S0 ([1/2]0, $2p'_1$) levels.

We have made extensive calculations and a detailed evaluation of both the transition probabilities (A_{ij}) and electron collision excitation cross sections (σ_i) concerning the 4*s* and 4*p* Ar I levels (Katsonis *et al.* 2008), in order to obtain recommended values for the needed data. Spontaneous emission and inelastic electron collisions are the two most important processes, not only for modelling purposes, but also because they define essentially the plasma spectra which are necessary for diagnosing the plasma and validating the models.

For calculations of A_{ij} a code (CbA) based in the Coulomb Approximation, proposed by Bates and Damgaard (1949) has been used, both in jK and LS coupling formulation. The jK coupling has given better results for Ar I, confirming our previous opinion that the neutral rare gases Ne, Ar, Kr and Xe are better described in jK coupling. These data were compared with intermediate coupling results from the SUPERSTRUCTURE programme (Eissner *et al.*, 1974) and from CATS, a Cowan code as adapted by J. Abdallah Jr *et al.* (1988). Also, experimental results were obtained in the University of Ioannina (Berenguer *et al.*, 2008) and compared to previous results described in the "*Handbook of Physics*" by H.M. Grosswhite and G.H. Diecke (1957).

Our global excitation rate curves for the 4s and 4*p* levels corresponding to Maxwellian distribution, are given in Figs. 2 and 3, compared with data contained in the Second edition of the book by Liebermann and Lichtenberg and (2005).

Evaluation of σ_i for 4s and 4p levels of Ar I was based on calculations with various types of approximations (DW, Born, relativistic DW), compared with the existing experiments and quasi-classical formulas.



Figs. 2 and 3 : Rate coefficients for 3p – 4s and 3p – 4p excitations.

The latter were previously proposed by Drawin (1967) and extended on the basis of CTMC calculations (Reports GA-22, GA-23, 2008 and GA-26, 2009). The obtained global excitation rate curves for the 4s and 4*p* levels for Maxwellian distribution, are given in Figs. 1 and 2. Comparison of the model theoretical results with the experimental spectra calls for a separate detailed

Collisional-Radiative (C-R) model of the Ar I. This C-R model calculates the individual population of each 4*s*, 4*p* level on the basis of the global 4s and 4*p* populations coming from the kinetic model and consequently allows for comparison with each experimental spectral line intensity and for the model validation.

2. Ar(4s) AND Ar(4p) WITH A LOW PLASMA COUPLING

The computation of the hydrodynamic parameters of the plasma flow in the arc-jet have been performed using a fluid description under several assumptions in order to determine the local parameters as static pressure, electron and heavy species temperatures, plasma density and plasma velocity . The plasma flow is assumed to be stationary because no arc foot movement is introduced on the anode surface and vortex flow movements due to the injection device is neglected due to the axial pressure gradient and turbulence effects are neglected in reason of the small values of the local Reynolds number. Morever, the erosion rate of cathode is weak enough to be negligible, the flow is supposed to be two-dimensional (r,z) and an azimuth rotation of the arc is not introduced, and the flow can be represented as a continuous fluid type and described by the Navier-Stokes equations without slip-wall conditions. Morever, the ionization involves the formation of only singly argon charged ions and the plasma is locally characterised by two kinetic temperatures e.g. electron temperature T_e and temperature T of ions and neutral atoms called heavy particles. The arc-jet is divided into two zones i.e. electric arc zone and expended plasma jet in the divergent part of the arc-jet. In this approach, the local and axial electric field is a function of co-ordinates r and z and a mean value can be calculated as

$$< E(z) > = \frac{I}{2\pi \int_0^{r_c} \sigma r dr}$$

where σ is the electric conductivity and r_c is the throat radius. The arc current I is an input data which is kept constant along the throat of the nozzle. expressed by Devoto R.S. and the average electron-neutral collision cross section is from Milloy H.B. et al.The local plasma velocity, mass density, mass and momentum balance equations are written in a cylindrical co-ordinate system as:

$$\frac{\partial}{\partial z}(\rho u) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v) = 0$$

$$\frac{\partial}{\partial z}(\rho u^2) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho u v) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial u}{\partial r}\right) - \frac{\partial p}{\partial z}$$

$$\frac{\partial}{\partial z}(\rho u v) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v^2) = \frac{2}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial v}{\partial r}\right) - \frac{2\mu v}{r^2} - \frac{\partial p}{\partial r}$$

where u and v are the axial and radial velocity components respectively, ρ the mass density, μ the viscosity and p the pressure. The mass density and pressure are related to particles densities and temperatures by the Dalton's law. According to the level of pressure in the nozzle, no-slip-wall conditions are introduced for the velocity. For singly ionised argon plasma in quasi-neutrality condition, only one electron continuity equation is needed for the plasma balance composition:

$$\frac{\partial}{\partial z}(n_e u) + \frac{1}{r}\frac{\partial}{\partial r}(r n_e v) = \frac{1}{r}\frac{\partial}{\partial r}\left(r D_a \frac{\partial n_e}{\partial r}\right) + S_e$$

where S_e is the electron source and D_a is the electron ambipolar diffusion coefficient from Devoto [4]. The electron energy balance equation, expressed in term of temperature instead of energy, is:

$$\frac{5}{2} n_e k\left(u\frac{\partial T_e}{\partial z} + v\frac{\partial T_e}{\partial r}\right) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\kappa_e \frac{\partial T_e}{\partial r}\right) + u\frac{\partial}{\partial z}(n_e k T_e) + v\frac{\partial}{\partial r}(n_e k T_e)$$
$$+ B(T - T_e) - Q_{rad} - S_e E_{ion} + \frac{j^2}{\sigma}$$

The energy balance of the heavy particles is written as:

$$\frac{5}{2} n_h k\left(u\frac{\partial T}{\partial z} + v\frac{\partial T}{\partial r}\right) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\kappa_h \frac{\partial T}{\partial r}\right) + u\frac{\partial p_h}{\partial z} + v\frac{\partial p_h}{\partial r} + Q_{elas}$$

where j^2/σ is the heat input by Joule effect, j the current density, σ the electric conductivity, Q_{rad} the radiation loss, Q_{elas} the energy exchange between electrons and heavy particles in elastic collisions, Q_{ion} the atoms ionization energy (or recombination energy), κ_e and κ_h are respectively the electron and heavy particles thermal conductivity. As presented, the balance equations are directly related to temperatures (Te,T) instead of energies (ε_e,ε_T)

Using the numerical code developed at IEPE (Poznan), these equations have been numerically solved to calculate plasma density, gas concentrations, pressure, temperatures (T_e,T) and velocity of the plasma flow. Electron density, Ar neutral and Ar ion (with a single ionisation) in ground states are introduced. The difference between the temperatures Te,T along the plasma axis in the throat and in the divergent part of the nozzle are presented on Fig.4.

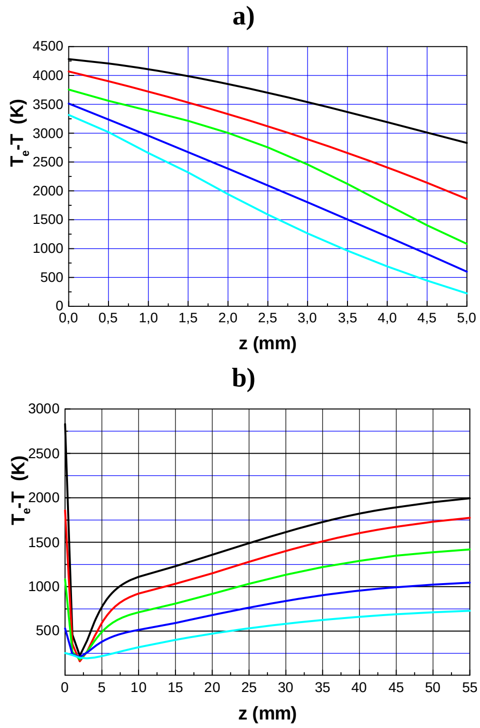


Fig. 4 : Difference between electron T_e and heavy particles T temperatures for a discharge current of —■— 60 A, —●— 80 A, —▲— 100 A, —▼— 120 A, —Λ— 140 A: a) in the throat, b) in the nozzle divergent part

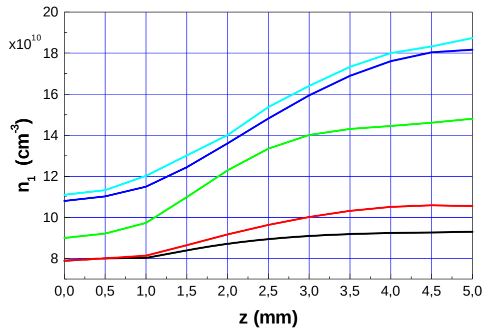
The populations of the states Ar(4s) and Ar(4p) are then calculated by using the obtained profiles of hydrodynamic parameters from the fluid code PAPYRUS.

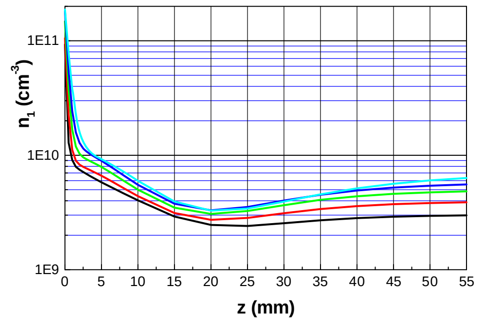
The Ar(4s) is formed by 4 levels: two metastables and two non stationary levels. In a first approximation, they are assembled in only common level for which the reaction rates are expressed. The same approach is used for Ar(4p) level formed of 12 levels.

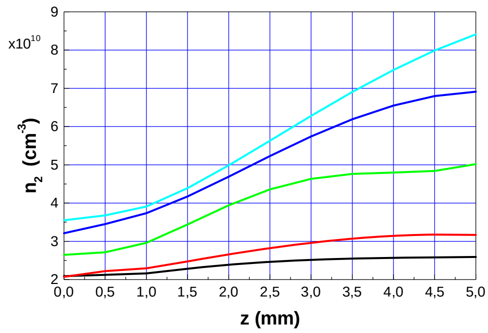
For Ar(4s), the excitation processes are due to electron collisions from the ArI GL (*$3p^6$*, neutral ground level), from Ar(4p) and from ArII GS (ion ground state). The rates of electron excitation have been calculated for each sub-level and then the global rate has been approximate as a function of the electron temperature (in the range 1-10eV). The de-excitation has been also expressed versus electron temperature. The probabilty of transition for de-excitation of Ar(4s) to Ar(4p) and ArI GL have been evaluated. Ionisation from Ar(4s) and a collisional desexcitation from ArII Gl are introduced.

For Ar(4p), the excitation processes are due to electron collisions from the ArI GL (*$3p^6$*, neutral ground level), from Ar(4s) and from ArII GL (ion ground state). The rates of electron excitation have been calculated for each of the twelve sub-levels and then the global rate has been approximate as a function of the electron temperature (in the range 1-10eV). The de-excitation by electron collisions has been also expressed versus electron temperature. The probabilty of transition for de-excitation of Ar(4p) to Ar(4s) has been evaluated.

The balance equations for the populations of Ar(4s) and Ar(4p) are solved at each point along the axis of the nozzle in the throat and in the divergent by using a steady state approximation and by using the calculated values of T_e, *n(ArI), n(Ar+)* = n_e by the Navier-Stokes code from IEPE. The Fig.3 presents the evolution of the populations of Ar(4s) and Ar(4p) for a discharge current in the range 80A-140A along the throat axis and the divergent axis. These two populations are increasing in the throat due to the input arc energy and are decreasing in the divergent. They are increasing with the arc power and the population of Ar(4s) is greater than Ar(4p) one (Fig.5).







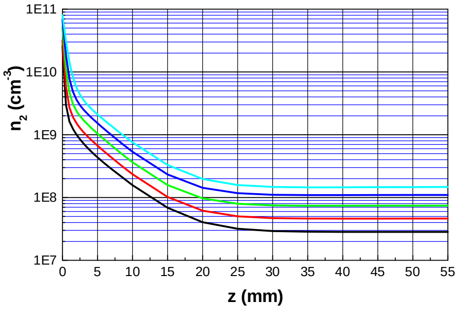


Fig. 5 : Population of Ar(4s) and Ar(4p) along the nozzle axis. Black – 60 A, red – 80 A, green 100 A, blue – 120 A, cyan – 140 A

3. Ar(4s) AND Ar(4p) WITH A HIGH PLASMA COUPLING

In parallel with upper investigations, calculations were made with two-way coupling between the different levels population variations and energy exchange in the flow. To do so, we solved as many equations of continuity as species (ie 4 in this case), the electron density being obtained from the neutrality condition of the plasma. The source terms of these equations are calculated from a pseudo-kinetic chemical two species reactions $\alpha' A+\beta' B \Leftrightarrow \alpha'' A+\beta'' B$ describing the production rate of mass

$$\omega_A = M_A(\alpha''-\alpha')(k_f[C_A]^{\alpha'}[C_B]^{\beta'} - k_b[C_A]^{\alpha''}[C_B]^{\beta''})$$

with M_A, M_B molar masses, $[C_A]$ and $[C_B]$ the molar concentrations, $k_f(T_g)$ and $k_b(T_g)$ constants of the chemical reaction. We use the Arrhenius formula to represent as a function of temperature. Only the 1-energy equation version of the code was used. It is therefore the global temperature T_g that is introduced in the Arrhenius formula. The heating of the flow in the throat is modeled by means of a uniform source term in the total energy equation. The set of conservation laws is complemented with the momentum equation for the mixture.

The results suggest two kinds of comments. First, the two-way coupling and modeling of the excitation by means of a pseudo kinetic seem to make sense at the aerodynamic scale. The population level (4s) is better reproduced than the (4p) one (Fig. 6). The explanation is probably to be found in the use of a single temperature. In fact, even when initialized to the temperature of heavy particles, the temperature tends to the electron temperature at the exit of the throat (Fig. 7). So its gradient is much higher. This behavior is reversed in the divergent and there Tg decreases very quickly but increases again nearby the exit of the nozzle to catch the temperature of heavy species.

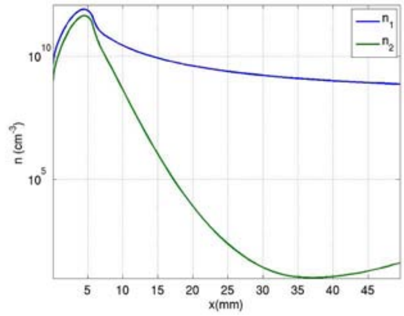


Fig. 6 : Density of Ar(4s) and Ar(4p)

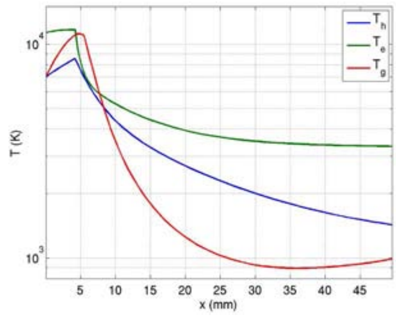


Fig. 7 : Comparing a single global temperature model with a two temperature one.

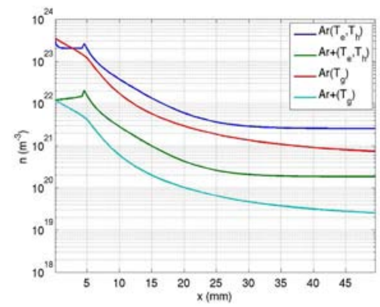


Fig. 8 Comparison of Ar and Ar+ densities obtained with the two approaches.

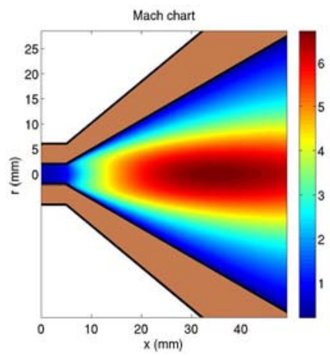


Fig. 9 The map of Mach number in the flow.

The densities of Ar and Ar+ are also sensitive to this fact (Fig. 8). This behavior must also be connected to the dynamical structure of the jet and hence the transport phenomena (Fig. 9).

CONCLUSION

Velocity, temperatures, pressure and density in the arc-jet have been previoulsy calculated using two Navier-Stokes codes taking into account dissipative effects and arc-gas exchanges for different re-entry problems (CO_2-N_2, N_2-CH_4, air). For the purpose of the present work we calculated the properties of an argon plasma in an arc-jet with Ar, Ar+, e and also with two levels Ar(4s) and Ar(4p) considered as supplemenatry species in the fluid codes. First results on the populations of Ar(4s) and Ar(4p) are presented. These encouraging results will be analysed in details in a next papers but they already seem to be consistent with expected behaviours.

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