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Numerical simulation of heat transfer and pressure distributions in micronozzles with surface discontinuities on the divergent contour

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ABSTRACT

This work describes two-dimensional numerical simulations of rarefied gas flows in convergent–divergent micronozzles. Array-arranged micronozzles with rectangular cross-section and convex–concave divergent shape are considered. The primary goal of this paper is to assess the sensitivity of the pressure, skin friction and heat transfer coefficients as well as the impact on the specific impulse due to the presence of surface discontinuities on the divergent contour of the micronozzles. The knowledge of thermal and mechanical loads present on the micronozzle surfaces is essential to predict operational conditions of a propulsive system. Because of the rarefied nature observed in micronozzle flows and the ability to deal with complex geometries, the Direct Simulation Monte Carlo method is employed to simulate the flow structure. For the conditions investigated, the computational results indicate a small dependence of the surface aerothermodynamic loads on the divergent curvature. On the other hand, these loads were strongly affected by the existence of singularities on the divergent contour, e.g., sharp corners. In spite of these findings, the specific impulse computed along the exit section was essentially the same for all investigated cases.

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1. Introduction

The recent tendency in the design of space systems has aligned to reduce the life cycle cost of space programs by means of a reduction in the complexity of satellite missions. Hence, one of the possible options concerns to the reduction in the mass of the whole system. The mass reduction will be possible only with a system miniaturization, i.e., a reduction in the satellite scale or in part of it. For this reason, concepts of micropropulsion based on microtechnologies have been developed in order to attend the requirements of future space missions.

The current state of semiconductor technology based on silicon has allowed the application of silicon plates in the manufacturing process of microscale devices. This manufacturing technique has been applied in the development of small scale systems, called as MEMS (MicroElectroMechanical Systems), and several others microdevices. Among the many MEMS applications one may cite the microactuators, microrefrigerators, microgenerators, micropumps and microunits of low thrust, where micronozzles are present.

The micronozzles normally provide a thrust of the order of microNewtons and miliNewtons. Such a force is required to provide an accurate attitude control of the satellite and to correct its

trajectory, which may suffer disturbances due to solar radiation pressure and drag influences. The thrust is typically obtained by the expansion of a gas through the convergent–divergent geometry that compose the micronozzle. Currently, the integration between micronozzles and different propellant feeding systems has been investigated $[1-3]$. Regardless the propellant storage phase, the fluid reaches the convergent micronozzle region in the gas phase and depending on the feeding system the gas may be at high or low temperatures.

Because of the gas-surface interactions, the micronozzle internal walls experience heat transfer and friction processes as well as pressure loads, which are even more significant at aerodynamic imperfections. Thus, the internal aerodynamic design of the micronozzle plays a primary role on the flow behavior and structural features. The knowledge of the thermal and mechanical loads present on the micronozzle walls is essential to select appropriate operational and conceptual features in the propulsive system, e.g., heat dissipation and ablative techniques, maximum burning time, bit impulse interval and so forth. Moreover, such an information may assist in the prediction of adverse impacts on spacecraft structures.

In spite of the growing number of successful applications of MEMS in scientific and engineering devices, nowadays there is only a minimum level of understanding related to the fluid dynamics in fluidic MEMS. As a consequence, several research studies have been conducted in order to understand the physical aspects of

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the micronozzle flows. Among others, these studies have investigated the micronozzle performance [\[4\],](#page--1-0) effects of 2D versus 3D geometries [\[5\]](#page--1-0), Reynolds number influence [\[6\],](#page--1-0) rarefaction effects [\[7\]](#page--1-0), surface temperature impact [\[8,9\],](#page--1-0) and different micronozzle arrangements [\[3,10\].](#page--1-0)

Most previous investigations have not focused on the influence of geometric imperfections, e.g., surface roughness [\[11\],](#page--1-0) contour discontinuities, and surface curvature, on the divergent micronozzle flow structure. Such imperfections may arise from manufacturing problems and, as aforementioned, they implicate on regions of intense aerothermodynamic loads. In this scenario, numerical simulations of rarefied gas flows in convergent–divergent micronozzles with discontinuous divergent contour are performed in the present study. The aim of this paper is to assess the sensitivity of the pressure, skin friction and heat transfer coefficients as well as the impact on the specific impulse due to the presence of surface discontinuities on the divergent contour of the micronozzles. Effects of different curvatures on the divergent surface are also investigated. Such results may be valuable in the design and development of micronozzles since near-optimal and critical conditions can be numerically predicted by means of only a fraction of the time and costs needed by experimental approaches.

In micronozzles, the molecular mean free path λ and the throat size t generally have the same order of magnitude. Based on the overall Knudsen number, $Kn = \lambda/t$, typically, the convergent region is within the continuum flow regime $Kn < 0.001$, the throat and divergent regions are within the slip flow regime $0.001 \le Kn \le 0.1$ and the transitional flow regime $0.1 \le Kn \le 10$, and the external flow is within the free molecular flow regime $Kn > 10$ [\[12\].](#page--1-0) In such a circumstance, modeling micronozzle flows with a continuum approach may lead to inaccurate results because such devices operate covering different flow regimes. Consequently, a kinetic approach must be employed to describe these flows.

2. Computational method

The DSMC method has become a reliable and efficient kinetic approach for modeling rarefied gas flows of engineering interest. This method was first proposed and applied by Bird [\[13\]](#page--1-0) to investigate homogeneous gas relaxation and shock wave structure [\[14\]](#page--1-0) problems. Subsequently, this method have been improved to study complex multidimensional problems in the fields of gas dynamics and physical-chemistry [\[15\]](#page--1-0). Typical applications include high altitude rocket plumes [\[16\]](#page--1-0), spacecraft propulsion [\[17\]](#page--1-0) and contamination, low-pressure plasma reactors for material-processing, reentry vehicles, and MEMS-based devices [\[18,19\]](#page--1-0). Although these applications encompass a wide range of spatial and temporal scales, they are united by the same underlying physics of moderate or high Knudsen number flows.

In the present account, the molecular collisions are modeled by using the variable hard sphere (VHS) molecular model and the notime counter (NTC) collision sampling technique. Simulations are performed with a non-reacting gas model, consisting to 76.3% of N_2 and 23.7% of O_2 . The VHS model parameters corresponding to these species are the same described by Bird [\[15\]](#page--1-0). The energy exchange between kinetic and internal modes is controlled by the Borgnakke-Larsen statistical model. Energy exchange between the translational and the internal modes of rotation and vibration are considered with constant relaxation collision numbers of 5 and 50, respectively.

3. Geometry definition

The geometry is based on a convergent–divergent micronozzle with rectangular cross-section. Such a device is considered as part of a micronozzle array [\[3,9,10\].](#page--1-0) By also considering a convex–concave divergent surface linked by an inflection point, the impact of different divergent shapes on the internal aerodynamic quantities are explored by changing the surface slope and curvature at the inflection point. Fig. 1 illustrates an array pattern composed of three identical micronozzles. In order to take advantage of the symmetries, it is assumed that the flow structure of this micronozzle array can be predicted by simulating only the pointed out regions with appropriate boundary conditions. Such a simplification yields tremendous computational saving. In addition, the convergent and buffer regions are also considered to avoid nonphysical behaviors in the divergent region [\[20,21\]](#page--1-0).

It is important to remark that results obtained by the present two-dimensional approach are consistent as long as the neglected micronozzle transversal dimension is considered much greater than the micronozzle throat and exit widths. In this situation, the current two-dimensional simulation can be considered a cross-section from the three-dimensional case extracted far enough from the flat walls, making their presence negligible.

Based on [Fig. 2](#page--1-0), region 1 represents the inlet chamber, regions 2–3 the convergent part, regions 4–7 the divergent part, and regions 8–9 the buffer zone. Due to the symmetry conditions, dimensions indicated by h mean a half size while the lengths are indicated by L. The subscripts in, c, t, d, e and b refer to the inlet, convergent, throat, divergent, exit and buffer sections, respectively.

The convergent part is composed of a surface inclined by a half angle θ_c that is tangent to a round shape of constant radius R_c . In analogous fashion, the convex surface of the divergent part is described by a round shape of constant radius R_d with slope θ_d at

Fig. 1. Schematic drawing of the simulated domain.

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