Design considerations for supersonic micronozzles

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Abstract: The next-generation of small satellites (‘nanosats’) will feature masses <10 kg and require miniaturised propulsion systems capable of providing extremely low levels of thrust. The emergence of viscous, thermal and/or rarefaction effects on the micro-scale can significantly impact the flow behaviour in supersonic micronozzles resulting in performance characteristics which differ substantially from traditional macro-scale nozzle designs. In this paper, we provide an overview of key findings obtained from computational studies of supersonic micronozzle flow and discuss the implications for future micro-scale nozzle design and optimisation.

Keywords: micropropulsion; micronozzle; nanosat; supersonic flow; microfluidics.


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1 Introduction

1.1 The need for micropropulsion: ‘nanosats’

Space agencies such as NASA and ESA, as well as defense agencies are currently pursuing the use of miniaturised satellites featuring masses <10 kg for the next generation of space missions. Commonly known as ‘nanosats’ – or ‘picosats’ for even smaller designs – these satellites will be capable of operating in distributed networks and performing mission objectives not currently achievable with traditional satellite architectures. Distributed spacecraft concepts such as formation flying represent a departure from traditional satellite philosophy which was based on a single, massive multi-functional spacecraft. These mission architectures also offer a number of advantages such as reduced mission cost (production and launch), increased flexibility and reliability, and improved data resolution (Moser et al., 1999; Weidow and Bristow, 1999). An excellent example of a distributed architecture is NASA’s planned Magnetospheric Constellation (MagCON). In this mission a network of roughly 50 nanosats will serve as in situ observing stations for studying the complex physics of the Earth’s magnetospheric handling of solar wind energy. The interested reader may find additional details and mission status updates on the MagCON Mission at the NASA/Goddard Space Flight Centre website.

As a result of the dramatically reduced size, nanosats will require unique and miniaturised propulsion systems to provide the extremely low levels of thrust and impulse necessary for orbital maneuvering and precise station-keeping.
More specifically, thrust levels of \(~1\ \mu\text{N}\) and impulse bits of approximately \(1–100\ \mu\text{N-s}\) are expected as design parameters (Blandino and Cassady, 1998; Pollard et al., 1999). The impulse ‘bit’ represents the minimum amount of impulse that can be delivered each time the thruster is fired; its magnitude is dependent upon both the level of thrust and the actuation speed of the thruster. From a controls perspective, it can be interpreted as a measure of the limiting resolution of spacecraft control capability from a given thruster at a given location. Propulsion systems must concurrently satisfy stringent constraints on mass, size and power consumption which traditional propulsion technology cannot meet (Mueller, 2000). To this end Micro-Electro-Mechanical Systems (MEMS)-based propulsion systems have been identified as potential solutions (Ketsdever and Mueller, 1999; Mueller, 2000). Typical operating parameters and constraints for micropropulsion schemes are discussed in Section 2.1.

MEMS-based thruster concepts are attractive because they offer the capability of effectively miniaturising traditional thruster designs for nanosat applications. The immediate design advantage is that the wealth of technical expertise accumulated from past satellite thruster design can be leveraged – however, additional micro-scale physics may need to be incorporated as will be demonstrated in this paper. Further advantages of MEMS-based propulsion system are numerous: they can be extremely small, with dimensions on the micron scale or smaller; their construction can be made extremely lightweight with simple components and low dead volume; and they can be reproduced in mass quantities with a low cost per device.

1.2 Brief overview of micropropulsion concepts

Over the past few years numerous and diverse micropropulsion initiatives have been undertaken by the government, industry and academia. The various approaches, all of which tend to have their unique benefits, have included liquid/solid chemical propellants and electric propulsion concepts, with somewhat of a focus on the latter. For the interested reader, a comprehensive survey of micropropulsion concepts under development can be found in Mueller (2000) and a review of micropropulsion systems targeted for formation flying applications can be found in Reichbach et al. (2001). In assessing the relative merit of a given approach, it is important to recognise that each mission specification will have its own set of unique constraints. Electrical-based microthrusters (e.g., pulsed-plasma thrusters/PPT, ion engines, field-emission electrical propulsion/FEEP) are capable of delivering extremely low thrust levels but currently are large in size and mass, and have relatively high power requirements. Solid propellant devices are limited primarily by their digital nature: once fired they are not reusable. These devices are therefore constructed in arrays (or ‘blister packs’) and necessarily have a pre-set number of firings in their lifetime. One such micropropulsion concept that is being developed at NASA/Glenn Research Centre is based on the laser-ignited decomposition of a solid monopropellant (de Groot et al., 1998; Reed, 2003).

Chemical propellants (e.g., hydrazine, hydrogen peroxide) have traditionally been attractive for satellites because they offer relatively high thrust-to-weight ratios owing to the inherently high energy density. A common measure of the energy density of a given chemical propulsion scheme is the specific impulse \(I_{sp}\), defined by

\[
I_{sp} = \frac{T}{mg_\text{th}}
\]
where $T$ is the thrust, $\dot{m}$ is the propellant mass flow rate, and $g_0$ is the acceleration due to gravity. The specific impulse thus represents the ratio of thrust produced per unit weight of propellant consumed. Another advantage of chemical thrusters is that they offer a greater range of total impulse, thrust level, and impulse bit than discrete solid propellant thrusters. Monopropellant schemes, in particular, are favoured because of their relative simplicity of design. Here, the energy source is derived from an exothermic catalytic chemical decomposition of a monopropellant fuel and avoids complications of fuel/oxidiser mixing necessary in bi-propellant schemes. The first prototype MEMS monopropellant micro-thruster was developed at NASA/Goddard Space Flight Centre in collaboration with the University of Vermont (Hitt et al., 2001) and used hydrogen peroxide as the monopropellant; the choice of hydrogen peroxide as a monopropellant in that work was largely motivated by the resurgence of interest in developing ‘green’ propellants.

Cold gas propulsion schemes are likewise attractive for design simplicity. The propulsion mechanism here is derived simply from the expansion of a pressurised gas from a reservoir. The primary disadvantage to cold gas systems is that the specific impulse is generally low due to the lack of combustion. Further, the thrust level and the efficiency diminish both over time as the pressure in the reservoir decreases with use and/or leakage. Nevertheless, cold gas systems have been identified for consideration in a number of future nanosat missions, including the ESA’s LISA-Pathfinder mission (Ziemer and Merkowitz, 2004).

1.3 Supersonic micronozzle design

A component ubiquitous to any chemical-based propulsion scheme is the converging-diverging nozzle (or a de Laval nozzle), whose role is to produce thrust by efficiently converting the pressure/internal energy of inlet gases into kinetic energy. Initial acceleration of a flow at subsonic speeds occurs in the convergent section and, for sufficiently high-pressure ratios and nozzle area contraction, it is possible to accelerate a flow to sonic conditions at the nozzle throat. The addition of a divergent section downstream of the throat enables further acceleration of the flow through supersonic expansion.

In traditional space propulsion applications, the combination of high speeds and moderate-to-large length scales result in very high Reynolds numbers – sufficiently large that inviscid analyses employed are as a first approximation. However, the importance of viscous effects in supersonic flows has emerged as a result of the development of micro-scale propulsion systems. With the characteristic length scales being considered for these new propulsion systems being on the order of microns to millimeters, the corresponding Reynolds numbers within the supersonic nozzles are $Re \sim 10^1 \sim 10^3$ and hence viscous effects can no longer be ignored. The scenario of low Reynolds number, supersonic flow represents an unusual flow regime, and one that has not been extensively examined in the fluid dynamics literature. In this regime, there is the usual thermo-fluidic complexity of a supersonic flow superimposed with subsonic viscous boundary layers extending from solid surfaces. At these low Reynolds numbers the viscous layer can occupy a sizable fraction of the divergent nozzle cross-section and, as a consequence, substantially impact the performance of the nozzle (e.g., thrust production). Aside from viscous forces, other important effects such as heat transfer and flow rarefaction may also be present on the micro-scale. The former becomes a concern as the thermal mass of the
flow is reduced and the surface area-to-volume ratio increases on the micro-scale. The latter introduces additional complications since gas kinetic (non-continuum) effects begin to emerge as the characteristic length scales begin to approach molecular mean free paths.

Taken together, the combination of viscous/thermal/rarefaction effects on the microscale can significantly impact the flow behaviour in supersonic micronozzles. Nozzles based on past macro-scale designs will exhibit performance degradations which are not predicted from traditional analyses. These degradations are especially significant for nanosat propulsion scenarios where fuel supply is inherently limited. From an engineering perspective, therefore, the accounting for these micro-scale effects is essential in the design of efficient micronozzles. In this paper, we provide an overview of the various engineering issues and challenges surrounding the design and fabrication of supersonic micronozzles. Given the experimental difficulty associated with micro-scale supersonic flow interrogation, detailed flow analyses are necessarily computational in nature. While some experimental works have also been reported (Ketsdever, 2002; Lempert et al., 2003; Ketsdever et al., 2005a) these have been generally limited to bulk thrust measurements without corresponding flow field data. Here, we summarise key findings from computational investigations of monoprellant and cold-gas propulsion schemes and discuss their consequences for efficient nozzle design.

2 Preliminary design considerations

2.1 Illustrative operating parameters and specifications

Owing to the substantially reduced size and mass, nanosats have unique propulsion requirements, including the ability to deliver extremely low levels of thrust and/or impulse for orbital maneuvering and attitude control. Extreme precision and accuracy of spacecraft control is essential for nanosats operating in formation-flying mission architectures. The primary method of attitude control is spin axis precession. In order to correct for perturbations such as solar radiation pressure or gravitational non-uniformities, the propulsion system must operate by firing low thrust, precise, and controlled impulse bits.

As an illustrative example of nanosat operating parameters, we consider the aforementioned NASA/GSFC prototype monopropellant microthruster, shown in Figure 1. The NASA/GSFC prototype is based on catalytic decomposition of a liquid monopropellant; primarily high-concentration hydrogen-peroxide\(^1\) (H\(_2\)O\(_2\)) or hydrazine (N\(_2\)H\(_4\)). The figure shows a photograph of a complete microthruster assembly and the labeled components of the device, respectively; the supersonic micronozzle has been outlined for clarity. A listing of target design specifications for this prototype is given in Table 1. A key parameter definition which will be used throughout this paper is the Reynolds number, which is defined here as

\[
Re \equiv \frac{\dot{m}L}{\mu A}
\]

(2)

where \(\dot{m}\) is the mass flow rate, \(L\) is a characteristic length scale (e.g., the nozzle throat diameter), \(\mu\) is the dynamic viscosity, and \(A\) is the cross-sectional area. We note in
passing that for the future ‘pico-sats’ being envisioned by the aerospace community and having masses less than 1 kg, the design constraints will be even smaller.

Figure 1  (Top) A photograph of the NASA/GSFC MEMS-based micro-thruster, placed atop a US penny to provide scale (Hitt et al., 2001). (bottom) A Scanning Electron Microscopy (SEM) image of the NASA/GSFC micro-thruster with key components labelled. The cover plate has been removed for clarity

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>Value/range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target thrust level</td>
<td>10–500 µN</td>
</tr>
<tr>
<td>Maximum specific impulse</td>
<td>180 s</td>
</tr>
<tr>
<td>Specific impulse efficiency</td>
<td>80%</td>
</tr>
<tr>
<td>Steady state inlet pressure</td>
<td>250 kPa</td>
</tr>
<tr>
<td>Inlet temperature</td>
<td>886 K</td>
</tr>
<tr>
<td>Mass flow rate</td>
<td>~0.015 kg/s</td>
</tr>
<tr>
<td>Throat area</td>
<td>9000 µm²</td>
</tr>
</tbody>
</table>
Design considerations for supersonic micronozzles

Table 1 Design parameters for the NASA/GSFC MEMS-based monopropellant supersonic micronozzle (continued)

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>Value/range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expansion ratio</td>
<td>6.22</td>
</tr>
<tr>
<td>Inlet mach No.</td>
<td>0.05</td>
</tr>
<tr>
<td>Exit mach No.</td>
<td>2.5–3.0</td>
</tr>
<tr>
<td>Reynolds number (throat)</td>
<td>&lt;1000</td>
</tr>
<tr>
<td>Impulse bit</td>
<td>1–100 µN s</td>
</tr>
</tbody>
</table>

Source: Hitt et al. (2001)

2.2 Design estimates via quasi-1D flow analysis

In the most basic terms, a supersonic micronozzle consists of a micro-machined duct with a varying cross-sectional area $A(x)$, where the $+x$-direction coincides with the flow direction within the duct. Under the ‘quasi-one-dimensional’ (quasi-1D) flow approximation, all flow variables are assumed to vary only with the streamwise position $x$ (and time if the flow field is unsteady). Variations across a given cross-section are considered negligible. Such an approximation is valid provided that the gradient $dA/dx$ is sufficiently small. The quasi-1D model is, of course, only an approximation of an actual 3D flow; however, it greatly simplifies analyses and often yields surprisingly good results in predicting basic nozzle behaviour. An overview of the quasi-1D nozzle model and its limitations can be found in most compressible flow references (e.g., Anderson, 2003).

The governing equations for the flow are obtained by one-dimensional approximations of conservation laws for mass, momentum and energy. Often the additional assumptions of inviscid, adiabatic flow are invoked and, as a consequence, the flow is regarded as isentropic throughout. From the conservation laws, one may derive an important isentropic relation between the cross-sectional area $A$ and the local Mach number $M$:

$$\left(\frac{A}{A^*}\right)^{\frac{2}{\gamma+1}} = \frac{1}{M^2} \left[ 1 + \frac{\gamma - 1}{2} M^2 \right]^\frac{\gamma+1}{\gamma-1}. \quad (3)$$

Here $M = V/a$ is based on the local velocity and speed of sound, $A^*$ is the area of the nozzle throat where sonic conditions exist, and $a$ is the isentropic speed of sound defined by

$$a^2 = \gamma RT \quad (4)$$

where $T$ is the static temperature, $R$ is the gas constant, and $\gamma = C_p/C_v$ is the ratio of the specific heats. For a prescribed nozzle profile $A(x)$, this ‘area-Mach relation’ yields the corresponding variation in the Mach number along flow direction. Further, for isentropic flow, it can be shown that the local thermodynamic properties (temperature $T$, pressure $p$, and density $\rho$) may be uniquely determined by the local Mach number according to the following:

$$\frac{T_*}{T} = 1 + \frac{\gamma - 1}{2} M^2 \quad (5)$$
\[
\frac{p_0}{p} = \left(1 + \frac{\gamma - 1}{2} M^2 \right)^{\gamma - 1} 
\]
(6)

\[
\frac{\rho_0}{\rho} = \left(1 + \frac{\gamma - 1}{2} M^2 \right)^{1/(\gamma - 1)} .
\]
(7)

Here, the subscript ‘0’ indicates the stagnation conditions \( M \to 0 \) corresponding to a specific flow state. In practice, these represent the inlet conditions of the gas(es) upstream of the nozzle inlet and, therefore, may be regarded as known states for the purposes of the nozzle modelling. In summary, for a prescribed nozzle profile \( A(x) \) and inlet conditions, the area Mach relation (3) and isentropic flow relations (5)–(7) are sufficient to completely determine the nozzle flow field under the quasi-1D model.

**Thrust, impulse and efficiency**

The ultimate deliverable for a supersonic nozzle in a propulsion application is the production of thrust and impulse. A control volume analysis of the nozzle indicates that the thrust produced at any moment in time can be well approximated by the momentum flux at the nozzle exit:

\[
T = \int_{A_{exit}} \rho \mathbf{u} \cdot \mathbf{n} dA = \dot{m} V_{exit} 
\]
(8)

where \( \dot{m} \) is the mass flow rate through the nozzle and \( V_{exit} \) is the average velocity at the nozzle exit plane. The mass flow rate is completely determined by the inlet conditions \( (p_0, T_0) \) and the nozzle throat area \( A^* \) according to (Anderson, 2003):

\[
\dot{m} = \frac{p_0 A^*}{\sqrt{T_0}} \frac{\gamma}{\gamma + 1} \left( \frac{2}{\gamma + 1} \right)^{(\gamma + 1)/(\gamma - 1)} .
\]
(9)

For transient operation, the total impulse during a single firing cycle of the thruster is given by

\[
I = \int_0^{t_b} T dt 
\]
(10)

where \( t_b \) is the total burn time or thrust duration of a single firing. Under the quasi-1D approximation, all force generated is necessarily in the axial direction (i.e., thrust). In actual 2D or 3D flows, this will generally not be the case and there will be performance reductions resulting from transverse velocity components at the exit. Thus, exit flow alignment is yet another consideration that is part of the overall supersonic nozzle design.

One common measure of the efficiency of a nozzle design can be obtained by normalising the specific impulse (1) by the corresponding value obtained from isentropic quasi-1D flow theory. For a given operating configuration, the nozzle efficiency \( I_{sp}^* \) is given by (e.g., Saad, 2003):

\[
I_{sp}^* = \frac{I_{sp}}{I_{sp}^{opt}}, \quad I_{sp}^{opt} = \rho g_0 \left[ \frac{2 \gamma R T_0}{g_0 (\gamma - 1)} \left( \frac{p_0}{p_0^{opt}} \right)^{\gamma - 1} \right] \left[ 1 - \left( \frac{p_0}{p_0^{opt}} \right)^{\gamma - 1} \right] \] 
(11)
where $p_e/p_0$ is the ratio between the exit pressure and the reservoir pressure at the nozzle inlet and $\dot{m}$ is determined from equation (9).

2.3 Micro-Nozzle geometry and fabrication methods

Area ratios and physical nozzle dimensions

The driving constraint of a micronozzle design is ultimately target thrust level, which is determined by the nozzle exit state and mass flow rate as given by equation (8). It is important to note that there is not a single flow state which produces a given level of thrust level, and thus other design constraints are required in order to determine a unique solution. Such additional considerations might include, but need not be limited to: the ambient back-pressure at the nozzle exit; the maximum allowable size of the nozzle; or the maximum mass flow rate $\dot{m}$ that the system can deliver. For micronozzles that are components of miniaturised propulsion systems, size may be the overriding concern and hence the exit area may provide the necessary additional constraint. Once the desired nozzle exit conditions have been identified, the nozzle area expansion ratio ($A/A^*$) is fixed by the area-Mach relation (3); moreover, the values of all the remaining thermodynamic ratios ($T/T_0, p/p_0, \rho/\rho_0$) are fixed by the isentropic flow relations (5)–(7). Actual areas and thermodynamic quantities are fixed once the inlet (stagnation) conditions and the nozzle throat (or exit) dimension are specified.

As an illustrative example, the NASA/GSFC described in Hitt et al. (2001) is designed to produce a thrust level in the range of 10–500 µN. This prototype featured a throat dimension of 90 µm and an exit area expansion ratio $A_{exit}/A^* \approx 6.2$ which produce an exit Mach number of ~3.4.

Ideal vs. actual nozzle profiles

The idealised nozzle profile $A(x)$ is one which provides the required area expansion ratios for supersonic flow and, concurrently, aligns the flow in the axial direction at the nozzle exit. This flow alignment minimises losses in thrust production associated with unwanted transverse velocity components. The traditional ‘bell-shape’ contoured nozzle accomplishes this task while maintaining isentropic flow conditions throughout the nozzle. Note that the profile of the isentropic bell nozzle cannot be obtained by quasi-1D theory. Rather, it is determined through the solution of expansion and compression wave propagation in the supersonic portion of the nozzle – typically this is done using the inviscid method of characteristics (e.g., Anderson, 2003).

While a contoured bell-shape profile may be the ideal case, there are two distinct and formidable design challenges on the micro-scale. First, contoured nozzles must be fabricated with high geometric precision in order to perform according to design. This level of fabrication precision has not been readily available over the last decade, and thus has proven to be a key consideration for the design of micronozzles. With continued improvements in micro/nano-fabrication techniques, it is likely that this obstacle will be overcome in the not too distant future. A second challenge to contoured micronozzle design rests within the design method itself. The theoretical profile of the ideal nozzle contour is obtained using inviscid flow theory, and thus ignores the effects of viscous boundary layers. While quite satisfactory on the macro-scale, this is wholly incorrect on the micro-scale. The correct contour calculation must include viscous effects; this not only complicates the overall calculation but, more importantly, the ideal
contour now becomes dependent on the Reynolds number of the nozzle flow. As an alternative to contoured nozzles, linear or conical nozzles are also common in thruster propulsion systems. A linear/conical nozzle features a supersonic section with a fixed expansion rate $dA/dx$ characterised by a divergence angle $\theta$ (see Figure 2, left). Such linear nozzle designs are attractive primarily for their geometric simplicity and the associated advantages in the fabrication process. Much of the current micropropulsion initiatives feature linear micronozzle designs.

**Figure 2** Schematics of the micronozzle geometries for two different configurations: (left) the linear micronozzle based on the NASA/GSFC prototype with expander half-angle $\theta$. The dimension $t$ is the thickness of the subsonic layer at the nozzle exit. (right) The linear aerospike nozzle, including the locations 20% and 40% truncations and the resulting “base” formation once the nozzle is truncated. All dimensions shown in this figure are in microns.

Regardless of the profile, one key difference between micronozzles and their macro-scale counterparts is their inherent 3D nature. Owing to the method of microfabrication (see below) the nozzles are inherently ducts with rectangular cross-sections. Conversely, all macroscale nozzles are conical in nature and thus the flows are 2D axisymmetric. The 3D nature of the flow can have substantial effects on the supersonic nozzle performance on the microscale; this point is discussed further in the Results section of this paper.

**Aerospike micronozzles**

An alternative micronozzle design has recently been proposed by Zilić and Hitt (2007) which is based upon the ‘linear aerospike’ design (Figure 2, right). Historically, aerospike nozzles were designed for Single-Stage-To-Orbit (SSTO) mission concepts, such as the NASA X-33 reusable launch vehicle. The distinguishing feature of the aerospike design is its ability to perform efficiently for a wide range of ambient back-pressures whereas traditional nozzles are only designed for a single ambient pressure. Back-pressure compensation is accomplished by utilising the dynamics of free-boundary reflection of the exiting jet flow to act as a virtual nozzle wall with a variable exit area ratio which adjusts with the ambient back-pressure. For the interested reader, further details can be found in Ruf and McConaughey (1997) and Sutton and Ross (2001).
For micropropulsion applications, there is little need for the pressure-compensation feature of the aerospike since the ambient conditions are those of either space or near-space. However, one can seek to leverage the fact that a virtual (free) boundary can mitigate viscous losses known to occur for internal micronozzle flows. The idealised spike geometry can be generated using the approach of Angelino (1964). In short, this inviscid approach combines Prandtl-Meyer expansion theory with the area-Mach relation for quasi-1D nozzle flow and determines the spike boundary as a particular streamline in the flow downstream of the nozzle throat. In practice, it has been experimentally observed that the majority of thrust for a macro-scale linear aerospike is generated over the first quarter of the spike. Consequently, it is common to truncate the spike to form a ‘plug’ nozzle to save weight. On the microscale, spike truncation also carries with it implications for boundary layer growth and flow separation.

**Microfabrication techniques**

Most micro-scale nozzles geometries are created from 2D planar patterns which are transferred to a substrate material (typically Si) via a photolithographic masking process. The nozzle is fabricated within the substrate by selectively removing the substrate material from unmasked regions; commonly this is accomplished via Reactive Ion Etching (RIE) or ‘deep’ RIE techniques. Whereas the RIE method is acceptable for etching depths on the order of 10 µm, the DRIE method enables etching depths in excess of 100 µm. Chemical wet etching is also possible, but is becoming less common because of its inherent limitations compared to RIE techniques. An alternative approach, and one which is becoming more widely available, is the use of ‘Focused Ion Beams’ (FIB) to mill out the pattern on the substrate. Regardless of the method, high precision is required in the fabrication process to ensure proper geometry is produced, including smooth nozzle walls. The nozzle is typically sealed by bonding a cover surface (e.g., Pyrex to provide optical access) to the substrate. Often anodic bonding is used to produce a permanent bond which can withstand a wide range of operating temperatures. To date, there has been little effort experimentally to provide for thermal insulation of the nozzle within the substrate. This may be an important area for future work given the potential significance of heat transfer during nozzle operation, as will be described later.

Most recently, Moll and Steciak (2006) have reported progress in the fabrication of micropropulsive devices within Low Temperature Co-fired Ceramic (LTCC) materials. The use of ceramic materials is very attractive for high-temperature propulsion systems, specifically those involving the use of solid propellants. LTCC materials also allow for a 3D multi-layer structuring and geometric featuring via conventional CNC milling. The primary limitation of this methodology at present appears to lie in the scaling of devices below the millimeter-scale.

### 3 Computational modelling

As indicated previously, the lack of experimental access to supersonic flows on the microscale requires that micronozzle design be based largely on computational and/or theoretical analyses of performance. In this section, we provide a brief overview of the numerical models used in simulating nozzle flows.
3.1 Continuum vs. rarefied flow regime

To this point, all discussion has tacitly assumed that the flow conditions are such that the continuum hypothesis remains valid within the micronozzle. The usual metric cited in arguing for (or against) the continuum assumption is the gas molecule (Kn), defined by $Kn = \frac{\Lambda}{L}$ where $\Lambda$ is the mean free path of the gas molecule and $L$ is a characteristic length scale. For supersonic nozzles the throat dimension is commonly chosen as the characteristic length scale. An alternative version of the Knudsen number which is of particular use in investigating supersonic flows is given by

$$Kn = \sqrt{\frac{\gamma \pi}{2}} \frac{M}{Re}$$

where, again, $M$ is the Mach number and $Re$ is the Reynolds number of the flow. While $Kn \rightarrow 0$ is the formal requirement for a continuum flow, in practical terms gas flows for which $Kn$ remains below a threshold value can be safely regarded as being within a continuum regime. The exact value of $Kn$ at which rarefaction effects begin to appear remains a matter of some controversy and generally depends upon the specifics of the flow under consideration; however, $Kn \sim 0.01 – 0.1$ is a representative range of values. At these and higher $Kn$ numbers, the breakdown in the continuum hypothesis is first manifested at the boundaries with the appearance of velocity and (if applicable) thermal ‘slip’ wherein a discontinuity occurs between the flow and the solid boundary where they interact. Mathematically, these modified boundary conditions take the form:

$$u_{slip} = Kn \frac{\partial u}{\partial n} + O(Kn^2) \quad T - T_{wall} = Kn \frac{\partial T}{\partial n} + O(Kn^2). \quad (12)$$

In practice, the flow within a supersonic micronozzle – and its plume – may span a wide range of Knudsen numbers encompassing continuum flow, highly-rarefied flows and all intermediate states in between. A key determinant, however, rests with the value of the ambient back-pressure. For cases where there is very low back-pressures (e.g., low Earth orbit or space) a significant portion of the flow field may be influenced by some rarefaction effects. Conversely at more modest back-pressures (e.g., high atmosphere operation) flow rarefaction may be quite negligible. In most high-altitude or space applications, the nozzle flow will always be under-expanded and the external plume will experience the greatest flow rarefaction. The degree of rarefaction can be quite severe, extending beyond the slip regime and bordering on the free molecular regime. In such cases, modelling efforts require the use of gas kinetic schemes such as Direct Simulation Monte Carlo (DSMC) or even Molecular Dynamics (MD). Detailed discussion of these methods are beyond the scope of this paper and the interested reader is encouraged to refer to the classic monograph by Bird (1994). It is important to note that, for supersonic flow, the level of accuracy required in the modelling of the plume region is really a ‘matter of interest’. For example, if there is need to study the interaction between gas particles in the plume with a spacecraft’s solid surfaces, then flow rarefaction cannot be ignored. On the other hand, if thrust production by the nozzle is the key item of interest, then the specifics of the supersonic plume may be of no real import.
3.2 Numerical methods for continuum flows

In the present work, the continuum-based flow analyses are focused on the performance of micronozzle flows featuring decomposed monopropellant fuels (hydrogen peroxide or hydrazine) after Hitt et al. (2001). The complete decomposition of the monopropellant fuel is assumed to have occurred upstream of the nozzle within the catalytic chamber. The decomposition of the hydrogen peroxide monopropellant proceeds according to the one-step reaction

$$2\text{H}_2\text{O}_2(l) \rightarrow 2\text{H}_2\text{O}(g) + \text{O}_2(g) + \text{heat} \tag{13}$$

whereas the hydrazine reaction occurs in a two-step process according to

$$3\text{N}_2\text{H}_4(l) \rightarrow 4\text{NH}_3 + \text{N}_2 + \text{heat} \tag{14}$$

$$4\text{NH}_3 \rightarrow 2\text{N}_2 + 6\text{H}_2 \tag{15}$$

In the numerical simulations, the thermophysical properties of these gas mixtures are assumed to be temperature-dependent and are calculated as a mass-weighted average of the mixture components.

Micronozzle performance is studied by implementing a continuum flow model for the geometry based upon NASA/GFSC prototype described in Hitt et al. (2001); see also Figure 1(d). The micronozzle expander half-angle is varied between 10° and 50° while all other geometric parameters are held constant. Two- and three-dimensional meshes have been developed in order to study the supersonic flow field in the micronozzle. The numerical meshes have been refined to a point where simulations are insensitive to further grid refinement. The throat and exit dimensions (90 µm and 560 µm, respectively) yield an area expansion ratio of ~6.2 and is a fixed parameter in the continuum portion of this study. The computational mesh is exactly identical in the inlet, converging, and exhaust regions. However, in order to maintain the constant area expansion ratio ($A_{exit}/A^*$) as the expander angle $\theta$ varies, the axial length of the expander section must also vary. The 2D meshes contain approximately 45,000–75,000 total elements whereas the 3D meshes contain approximately 1.5–2 million elements.

The micronozzle flow field is governed by the compressible Navier-Stokes equations which are solved using a coupled implicit solver for all simulations. The governing conservation equations for mass, momentum, and energy are given by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \tag{16}$$

$$\frac{\partial}{\partial t} (\rho \mathbf{V}) + \nabla \cdot (\rho \mathbf{V} \mathbf{V}) = -\nabla p + \nabla \cdot (\tau) \tag{17}$$

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\mathbf{V} (\rho E + p)) = \nabla \cdot (k \nabla T + (\tau \cdot \mathbf{V})) \tag{18}$$

$$E = h - \frac{p}{\rho} + \frac{V^2}{2} \tag{19}$$

$$\tau = \mu \left( (\nabla \mathbf{V} + \nabla \mathbf{V}^T) - \frac{2}{3} \nabla \cdot \mathbf{V} \mathbf{I} \right) \tag{20}$$
In these equations, $E$ is the specific energy, and $p$ is the absolute local pressure, $\mu$ is the fluid viscosity, $k$ is the thermal conductivity, $T$ is the static temperature, $h$ is the enthalpy, and $\tau$ is the viscous stress tensor. The system is closed by the ideal gas law equation of state 

$$p = \rho RT.$$  

The inlet flow boundary conditions are based on the original NASA/GSFC design specifications and the thermophysical properties of the decomposed monopropellant. The inlet temperature is equal to the fully decomposed adiabatic flame temperature of 85% concentration H$_2$O$_2$ and is set at 886 K. The same inlet temperature is used for the N$_2$H$_4$ simulations since it, coincidentally, correlates well with the flame temperature of fully decomposed N$_2$H$_4$. The inlet pressure is varied to achieve different mass flow rates (and Reynolds numbers) according to equation (9). A constant backpressure of 1.0 kPa is imposed as a pressure outlet boundary condition in order to assure that the flow remains within the continuum regime. In this numerical scheme, the ambient pressure is imposed only on the outlet boundary locations where the flow is subsonic; for supersonic regions, the pressure and all other flow quantities are extrapolated from the flow in the interior via Riemann invariants. No-slip boundary conditions are imposed at the nozzle walls in accordance with continuum theory; this can be justified a posteriori via a Knudsen number analysis of the flow field for the ambient pressures used in the simulations.

3.3 Numerical methods for rarefied flows

For micronozzles at large Knudsen numbers, Kn > 0.01 at the throat, the macroscopic description of gas flows based on continuum hypothesis – such as Navier-Stokes equations – breaks down and a numerical method capable of describing non-continuum, rarefied gas flows needs to be applied. The DSMC method, proposed by Bird (1994), is a statistical approach for the solution of the Boltzmann equation describing the spatial and temporal variation of the velocity distribution function due to the main physical processes of molecular motion: free flight, intermolecular collisions and action of an external force. In the DSMC method the velocity distribution function and gas macroparameters, such as density, flow velocity and temperature, are determined through simulation of model particles that move and collide with each other and solid surfaces. Typically, thousands or millions of model particles are used in DSMC. The number of real gas molecules is, of course, much larger: there are about $2.5 \times 10^{16}$ air molecules in each cubic millimeter at standard atmospheric conditions. The ratio of the number of model particles to real gas molecules, denoted $F_{NUM}$, is an important parameter of a DSMC simulation. The interested reader can find a detailed explanation and discussion of the DSMC in Bird (1994); here, we will briefly describe the main principles of the method.

Spatial discretisation and sampling

The flow domain of interest is divided into discrete cells that are used for spatial averaging of molecular properties. The state of gas at any moment in a location inside the flow domain is determined by averaging the molecular properties, such as mass, momentum and energy, over all model particles within the corresponding cell. The computational mesh should be fine enough so that the change in gas properties
across each cell is small, i.e., the cell size should be smaller than the local mean free path. When the cell size in a DSMC simulation is too large, macroscopic gradients are typically underpredicted and the solution corresponds to an artificially larger Knudsen number.

**Time discretisation**

The fundamental principle of the DSMC method is the splitting of the dynamics of molecular motion during a time step $\Delta t$ into two sequential stages: freeflight of molecules and intermolecular binary collisions. This approach is justified for ideal dilute gases where the time averaged potential energy of molecules is negligible compared to their kinetic energy and all collisions can be considered as instantaneous. The time step in the simulation is selected such that $\Delta t < \min(\tau_c, \tau_{res})$, where $\tau_c$ is the mean time between collisions, $\tau_{res}$ is the mean residence time in a cell, so that the molecules do not cross more than one cell during a time step.

**Molecular free flight**

The process of free flight is simply modelled by changing the positions of all model particles according to the time step and the molecular velocity as

$$\vec{c}_i(t+\Delta t) = \vec{c}_i(t) + \vec{v}_i \cdot \Delta t$$

where $\vec{c}_i$ and $\vec{v}_i$ are position and velocity of a particle $i$. Similarly, model particles are accelerated due to the action of external force $F$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\vec{F}}{m} \cdot \Delta t$$

where $m$ is the molecular mass.

**Binary collisions.**

Modelling of binary collisions in DSMC involves two steps:

- sampling of an appropriate number of collisions in each cell
- sampling of the post-collisional velocities for each pair of colliding particles.

The time between consecutive collisions, $\tau_c$ can be simulated for each cell from the exponential distribution $\nu \exp(-\nu \tau)$ where $\nu$ is the collision frequency. The acceptance-rejection method can be applied to sample the time between collisions using a maximum collision frequency $\nu_{max}$ as

$$\nu_{max} = \frac{N_c(N_c-1)}{2} \frac{F_{rel}}{V_c} \sigma(v_i) v_i$$

where $N_c$ is the number of model particles in the cell with the volume $V_c$, $v_i = |\vec{v}_i - \vec{v}_j|$ is the magnitude of the relative velocity between particles $i$ and $j$ and $\sigma(v_i)$ is the collision cross-section which depends on the binary interaction potential.

**Boundary conditions**

At each time step, the boundary conditions of the flow problem are modelled through particle injection at the domain boundaries and collisions with solid surfaces.
One of the most widely used gas-surface interaction models, the specular/diffuse Maxwell model, assumes that a fraction \((1 - \alpha)\) of particles colliding with a wall are reflected specularly while the remaining fraction \(\alpha\) experience a diffuse reflection. In the diffuse reflection the particle velocities are distributed according to the Maxwellian distribution corresponding to the wall temperature. This parameter \(\alpha\) is also referred to as the tangential momentum accommodation coefficient.

The majority of published modelling results on rarefied flows in nozzles were obtained using the DSMC method. An alternative numerical method was used, for example, in Chung et al. (1995) where a deterministic, discrete-ordinate solution of an approximate form of the Boltzmann equation was developed. The advantages of using the DSMC method to study micronozzle flows involving mixtures of non-perfect gases are: comparative simplicity of implementation even in three-dimensional form; the possibility of using various physical models for particle interactions, internal energy transfer and chemical reactions, and a relatively straightforward and efficient parallelisation. However, the computational cost of the DSMC simulations increases with decreasing Knudsen number. A modification of the DSMC technique for low Knudsen number nozzle flows has been suggested in Titov et al. (2006) based on the use of collision limiters in dense parts of the flow and outside of the wall boundary layer.

### 3.4 Approaches for the continuum-transition regime

We conclude this discussion of numerical methods with a brief summary of approaches developed for the so-called ‘transitional’ flow regime. Although this topic is not formally featured in the results of this paper, we provide this overview here for the sake of completeness and as additional information for the interested reader. The transitional regime is characterised by the emergence of non-negligible flow rarefaction effects and deviations from local thermodynamic equilibrium. Knudsen numbers corresponding to transitional flows lie (conservatively) in the range of 0.01–0.10. For weakly transitional flows, the continuum-based model (Navier-Stokes) can be adequately corrected by imposing the velocity and thermal slip conditions in equation (12). This correction comes with little, if any, computational penalty and is a straightforward means for extending the useful range of Navier-Stokes solvers up to \(Kn \approx 0.1\) (Hadjiconstantinou, 2006).

This is an attractive alternative – especially for design purposes – to methods such as DSMC which carry much higher computational costs and can represent an ‘overkill’ for weakly rarefied flows.

For still higher Knudsen numbers in the transitional regime, it is possible to extend the usable range of the continuum-based equations to \(O(Kn^2)\) through the incorporation of additional linear and nonlinear stress and heat transfer terms (Agarwal et al., 2001). Known generally as the Burnett equations, this model is derived from a second-order Chapman-Enskog expansion of the Boltzmann equation with the Knudsen number as a small parameter. Although the extending the useful range of continuum-based modelling, the Burnett equations have been shown to exhibit numerical instabilities at higher Knudsen numbers and, in fact, produce violations of the second law of thermodynamics (Comeeaux et al., 1995). The sensitivities associated with the Burnett approach render its usage for design purposes somewhat suspect, and its relative advantage compared to the more computationally expensive DSMC methods is not definitive.
4 Key findings from nozzle flow simulations

4.1 Steady-state operation

Much of the research to date has focused on the interaction of viscous forces, rarefaction effects and micronozzle geometry in an effort order to better understand and quantify performance characteristics. In this section, we focus on the impact of viscous forces; the discussion of rarefaction effects is considered in Section 4.2. The majority of the research literature has dealt with 2D planar or axisymmetric flows under steady-state conditions. Given the experimental challenges associated with micro-scale supersonic flow interrogation, the vast majority of the analyses have been computational in nature.

Within the aerospace literature, Bayt and Breuer (2001) were among the first to examine micronozzle flow and to identify the key role that viscous effects can play. In short, the low Reynolds numbers of these flows – typically less than 1000 – permit the growth of relatively thick subsonic layers near the walls within the supersonic expansion section of the nozzle. These layers can occupy a significant portion of the nozzle exit, effectively restricting the flow and reducing thrust production and nozzle efficiency. In an effort to compensate for the viscous subsonic layers, propulsion researchers have considered widening the expansion angle $\theta$ of the diverging section of the micronozzle (see Figure 1). Doing so, however, introduces geometric losses linked to increased non-axial velocity components at the micronozzle exit. Here too, the subsonic layer contributes to thrust reduction. The subsonic layer functions as a ‘conduit’ for ambient conditions downstream of the nozzle exit to interact with the flow within the nozzle, which is not possible for inviscid supersonic flows. For under-expanded micronozzle flows which would be typical of a space or near-space environment, premature flow turning will occur via an expansion fan which forms at the nozzle exit corners. This further increases the non-axial components of the exit velocity vector.

4.1.1 2D flow behaviour

To illustrate the impact of viscous forces on performance, we present key results obtained for 2D numerical simulations of the steady-state operation of the NASA/GSFC prototype micro-thruster device described in Hitt et al. (2001). While the simulation data is somewhat case specific, the findings and issues that arise are germane to most micro-scale nozzles. Simulations have been performed for expander half-angles in the range of $\theta = 10–50^\circ$ for throat Reynolds numbers less than 1000 and adiabatic conditions. Shown in Figure 3 is a plot of the thrust production vs. $\theta$ for cases of decomposed hydrogen peroxide and hydrazine monopropellants.

Referring to Figure 3, a notable reduction in thrust output is observed as the expander half-angle is increased above 30°. This is a direct consequence of expander geometry. For large expander angles, the flow follows the walls in the expander and thus a sizable component of the velocity vector exits the nozzle in the transverse direction. This results in a significant reduction of axial momentum flux and a corresponding decline in thruster performance. For small expander angles, transverse velocity components due to expander geometry are reduced, but at the expense of increased nozzle length in order to maintain the desired area expansion ratio. As the expander angle is decreased below 30°, viscous forces acting over the lengthened expander section begin to dominate nozzle performance. The subsonic layer acts to restrict the flow and reduce the effective exit
These factors combine to represent a performance trade-off between viscous and geometric effects as described further in Louisos and Hitt (2005).

**Figure 3** Performance results for 2D and 3D simulations of the NASA/GSFC microthruster nozzle operating at steady-state with adiabatic walls. The throat Reynolds number is approximately 800. The results have been normalized by quasi-1D theory. The H\textsubscript{2}O\textsubscript{2} micronozzle exhibits a maximum performance for θ ~ 30°. Note that the N\textsubscript{2}H\textsubscript{4} results do not exhibit a clear maximum nor do they experience a thrust loss at small angles. In the 3D simulations the 30° optimum half-angle becomes more pronounced although the thrust level is reduced by viscous effects.

To provide additional insight into the nature of the viscous effects, the subsonic boundary layer in the nozzle expander can be examined. Figure 4 shows the viscous subsonic boundary layer in the 30° expander half-angle for a H\textsubscript{2}O\textsubscript{2}-based micronozzle. Forming at the throat, the subsonic layer grows with axial distance. The steady-state subsonic layer thickness at the nozzle exit has been quantified as a function of expander half-angle in Figure 5. As the expander angle is decreased, the subsonic layer grows to occupy a larger percentage of the nozzle exit area, up to 15% for decomposed H\textsubscript{2}O\textsubscript{2} and up to 8.5% for the lower viscosity case of decomposed N\textsubscript{2}H\textsubscript{4}. For cases of smaller expansion angles, the corresponding length of the expander increases allowing the subsonic layer to grow as the flow moves further downstream. This scenario is directly responsible for the reduction in performance of the micronozzle at small divergence angles. For larger expander angles, the subsonic layer thickness again increases proportionally. Here the flow is forced to turn sharply at the throat as it enters the expander section. The high speed bulk flow is unable to turn efficiently and a thick subsonic layer results near the wall boundary. However, owing to the low Reynolds number regime, no flow separation is observed here.

It is clear that the interplay between viscous effects and geometry is a complex one and must be fully characterised for the efficient design of high-performance micronozzles. In short, with the operating conditions specified for the micro-thruster nozzle, trade-offs between the size of the subsonic layer and geometric losses due to non-axial flow components result in an optimal linear expander half-angle. For H\textsubscript{2}O\textsubscript{2}-based micronozzles, this angle is found to be approximately 30°, which is significantly larger than half-angles of around 15° typically used in macro-scale conical.
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thrusters (Humble et al., 1995). While the N₂H₄-based micronozzle does not exhibit a distinct maximum thrust output corresponding to an optimal geometry, it appears that the most effective half-angle is in the range of 25° and less.

4.1.2 3D effects

Much of the modelling efforts in the aerospace literature to date have focused on approximate 2D planar (or axisymmetric) geometries, owing largely to the 2D nature of patterning associated with typical microfabrication procedures. These approximations have also been pursued for very practical purposes as well: the computational resources needed for fully-3D calculations are quite expensive and require access to high-performance computing clusters—particularly in cases of transient flows and flows with rarefaction. In reality, MEMS-based supersonic nozzles will necessarily be 3D ducts having rectangular cross sections as a result of RIE or milling performed in the fabrication process. The validity of the 2D approximation improves with ‘deep’ nozzles and, conversely, worsens for ‘shallow’ nozzles; in practice, the latter case is much more likely and the depth dimension may be substantially smaller than the nozzle width at the exit plane. One would therefore posit that viscous boundary layer growth from the upper and lower solid boundaries of a 3D nozzle should be of similar importance as the side-wall boundary layers studied in the 2D simulations.

Figure 4  Mach number distribution for a H₂O₂-based micronozzle flow at a low throat Reynolds number of 30. The shaded portion of the lower half of the figure shows the extent of the subsonic region for this case.
Figure 5 A plot of the fraction (%) of the micronozzle exit area occupied by the viscous subsonic boundary layer for varying expander angles; the simulation conditions are the same as in Figure 3. The 3D simulations are bounded by walls on four sides and as such, the subsonic layer occupies a large percentage of the exit area. Note that the maximum thrust output does not directly coincide with the smallest subsonic layer

To illustrate the importance of 3D effects, the nozzle performance for the 3D NASA/GSFC H$_2$O$_2$ prototype under steady-state, adiabatic conditions has been characterised and compared with 2D results (see Figure 3). The simulations assumed a micronozzle depth of 150 µm and varying expansion angles; all other simulation parameters were identical to the 2D studies. The results have again been normalised by quasi-1D inviscid theory. Overall, one observes roughly a 5–7% reduction in thrust production in comparison to the 2D predictions. This difference is due to the fact that the 2D model does not account for subsonic boundary layer growth on the upper and lower walls of the micronozzle. There is a corresponding increase, roughly two-fold, in the percentage of the subsonic layer occupying the nozzle exit plane for 3D flow, as shown in Figure 5. Unlike the 2D model, the subsonic layer coverage decreases monotonically with increasing expander angle – a consequence of the boundary layer growth on the upper and lower walls. For small expander angles, the expansion section will have the greatest length so as to achieve the prescribed area expansion ratio; this length allows for the maximum boundary layer growth on all walls. The opposite is true for large expansion angles.

As with the 2D model, there is again a trade-off between viscous losses and geometric losses for a given expansion angle. For the simulations considered, the 3D H$_2$O$_2$ model indicates a performance-maximising expansion angle of ~30° which is virtually the same as for the 2D case. It is noteworthy to mention that the optimising angle is noticeably more pronounced in 3D (see Figure 3).

4.1.3 Linear aerospike micronozzles

As discussed earlier, the ansatz for examining a linear aerospike configuration for a microscale thruster is derived from its potential to allay viscous losses known to occur
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for internal micronozzle flows. To date, no analyses of aerospike nozzle performance on the micro-scale (i.e., low Re) have appeared in the aerospace literature.

Numerical simulations have been performed for decomposed H₂O₂ flow at varying Reynolds numbers in both full-spike and truncated spike geometries; for the latter situations, 20% and 40% truncations have been examined. The subsonic inlet geometry and the throat dimension was identical to that used in the 2D NASA/GSFC model simulations. The exit flows ranged from over-expanded at low mass flow rates to under-expanded at higher flow rates. The flow behaviour on the micro-scale (Figure 6) exhibits many of the same general flow features reported in the aerospace literature for large-scale aerospike nozzles (Ito et al., 1999). At low Reynolds numbers, a notable subsonic boundary layer forms along the length of the spike (see Figure 6), similar to that observed for the linear micronozzles. For sufficiently low Reynolds numbers the subsonic layer can become sufficiently thick as to severely restrict the flow downstream of the throat.

Figure 6 Structure of the flow field for under-expanded flow in a linear aerospike micronozzle; for purposes of clarity, only a zoomed-in portion of the entire domain is shown. The top half of the figure is a contour map of Mach number distribution, including an iso-surface of $M = 1$ which defines the subsonic boundary layer. The lower half of the figure shows the streamlines within the flow field.

Thrust production has been calculated for full and truncated (20%, 40%) aerospikes for a Reynolds number of ~800 and compared with predictions from inviscid simulations (Table 2). The variation in thrust data results from two sources. First, the decrease in thrust as the aerospike is truncated is expected from inviscid theory since the effective area expansion ratio at the spike end is reduced. However, the viscous flow calculation shows a much more severe decrease in performance for truncated aerospikes. Detailed examination of the flow field shows that it is the joint combination of the viscous subsonic layer and subsonic flow turning at the end of the truncated spike that is responsible for the notable reduction in performance.

The use of truncated aerospikes on the macro-scale is a practical design consideration in which substantial weight savings can be obtained with modest reductions in thrust.
production, as evidence by the inviscid results here. On the micro-scale, the flow separation effects at the lower Reynolds numbers result in much more severe penalties in performance—moreover, the savings in weight associated with a truncated aerospike is virtually negligible for a MEMS device. Thus, from a design perspective, it appears that only full (or nearly so) aerospike configurations should be considered.

Table 2  
<table>
<thead>
<tr>
<th></th>
<th>Full spike (100%)</th>
<th>40% truncated spike</th>
<th>20% truncated spike</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscous</td>
<td>29.56</td>
<td>20.94</td>
<td>18.81</td>
</tr>
<tr>
<td>Inviscid</td>
<td>35.72</td>
<td>29.69</td>
<td>27.07</td>
</tr>
<tr>
<td>Thrust ratio</td>
<td>0.828</td>
<td>0.705</td>
<td>0.695</td>
</tr>
</tbody>
</table>

4.1.4 Summary of steady micronozzle performance

As indicated previously, one common measure of the efficiency of a given nozzle design under steady operation is the normalised specific impulse $I_{sp}$ defined by equation (11). To summarise the findings of this section, we present the value of $I_{sp}$ as a function of the throat Reynolds number for various 2D and 3D nozzle configurations in Figure 7. Also shown on this figure are the results for rarefied flow calculations, which are discussed in the next section.

Figure 7  A summary plot depicting calculated micronozzle efficiencies $I_{sp}$ as a function of the throat Reynolds number
For the 2D linear micronozzle configurations, it is seen that efficiency is quite poor at low throat Reynolds numbers (Re \( \leq \sim 50 \)). However, for Reynolds numbers greater than \( \sim 200 \) there are relatively minor variations in the efficiency, which exceeds 90%. As mentioned earlier, an expansion angle of \( \sim 30^\circ \) gives maximum efficiency, yet for Re \( > 600 \) the results are nearly indistinguishable from the 20\(^\circ\) nozzle. The existence of an ‘optimal’ expansion angle appears to be most pronounced for throat Reynolds in the range of 100–200, where it is seen that the maximum performance is actually attained for a wider 40\(^\circ\) geometry. The degradation in performance for 3D linear micronozzles is also apparent in this figure, where a 6–8% reduction in efficiency is found when compared to the 2D predictions.

The full linear aerospike appears to deliver efficiencies comparable to the 2D linear micronozzles and superior to 3D linear micronozzles. While fully 3D simulations are still needed for the linear aerospike characterisation, the results are promising. Inclusion of 3D effects are unlikely to incur the level of losses as with the linear micronozzles since the additional boundaries will not be solid walls, but rather ‘free boundaries’. In contrast, the truncated aerospikes should show significantly reduced efficiencies, suggesting that such configurations may not be well suited for micro-scale nozzle design.

### 4.2 Rarefaction effects

The DSMC method has been used by Ivanov et al. (1999), Alexeenko et al. (2002) and Liu et al. (2006) to perform non-continuum analyses of milli-/micro-nozzle flows in order to examine the influence of rarefaction effects on performance. The work has found that for Knudsen numbers of \( Kn \sim 0.01 \), gas-surface interactions have a strong influence on the flow in the diverging section of the nozzle. As such, a large portion of the flow remains subsonic along the nozzle expander walls. This causes an overall reduced Mach number at the nozzle exit and decreased thrust production.

Comparisons have also been made between micronozzle flowfield and performance predictions obtained by DSMC and Navier-Stokes continuum models (Alexeenko et al., 2002; Liu et al., 2006) for the throat Reynolds numbers ranging from 40 to 400. Figure 8 shows a comparison of the Mach number flowfields calculated using the DSMC and Navier-Stokes approaches for a cold gas expansion through a conical nozzle at the throat Reynolds number of 400. The DSMC and no-slip Navier-Stokes solutions exhibit good agreement within the nozzle and differences between the two methods are confined to the vicinity of the nozzle exhaust plume, specifically the corners of the nozzle exit. For lower Reynolds numbers, the use of slip boundary condition in the Navier-Stokes model, improves the agreement between the two methods. However, the continuum-based approach breaks down in the flow regions where the local Knudsen number is larger than about 0.05 (Liu et al., 2006).

Another manifestation of the rarefied effects in micronozzles, is the thermal non-equilibrium, i.e. the difference between internal and translational energy modes of molecules. Such a non-equilibrium occurs in nozzle expansions at high Knudsen numbers due to insufficient number of intermolecular collisions that a gas molecule experiences while accelerating through the nozzle expander. Figure 9 shows the distribution of translational, rotational and vibrational temperatures of nitrogen gas expanding through a conical micronozzle at the throat Reynolds number of 400. The stagnation temperature of the flow in this case is 300 K and the vibrational energy mode stays effectively frozen throughout the nozzle. The difference between the rotational and translational
temperatures becomes significant in the nozzle exhaust plume. Since the main function of a converging/diverging nozzle is to convert the energy of thermal motion of molecules (translational, rotational and vibrational) into the bulk flow kinetic energy, the delay in the rotational and vibrational energy relaxation represents a loss factor for a micronozzle at low Reynolds numbers. The reduced efficiencies associated with the flow rarefaction are demonstrated in Figure 7.

**Figure 8** Mach number contours in a conical micronozzle at the throat Reynolds number of 400 calculated by the DSMC method (top) and Navier-Stokes equations with no-slip boundary conditions (bottom).

**Figure 9** Vibrational, rotational and translational temperatures in a conical micronozzle at the throat Reynolds number of 400 calculated by the DSMC method.

Experimental and numerical investigations of helium flow in conical micronozzles in highly rarefied regime was conducted in Ketsdever et al. (2005b). In that study the throat Reynolds number ranged from 0.16 to 200, resulting in the strong rarefaction effects in both converging and diverging nozzle sections. The thrust measurements for a conical nozzle and a thin-walled orifice of the same diameter as the nozzle throat were obtained using a nano-Newton thrust stand (Jamison et al., 2002). For throat Reynolds numbers less than 100, the thrust of the conical nozzle is less than that of the orifice, although the converging/diverging nozzle has a larger specific impulse compared to the orifice for the whole range of Reynolds numbers. In general, the DSMC results agree with the experiment. A few percent difference between the experiments and numerical modelling
was attributed to the uncertainty of surface roughness caused by the machining process. The DSMC results obtained with a proposed anti-specular gas-surface interaction model show a better quantitative agreement with experiment than the standard diffuse/specular Maxwell model.

4.3 Transient flow

In practice, nanosat station-keeping and attitude control is accomplished through the application of discrete impulse ‘bits’ resulting from the transient firing of the microthruster. The ability to precisely predict and control the impulse bit delivered during a firing is evidently of great importance from an operations standpoint. The thruster firing for a chemical-based (liquid/gas) system essentially involves three phases: start-up, a period of steady-state operation, and a shut-down sequence. Current design estimates of micro-valve actuation of the propellant flow is on the order of milliseconds.

For a typical microthruster firing, the micro-valve is initially closed and there is no flow through the nozzle. As the valve opens, a pressure gradient is established across the nozzle and the corresponding mass flow through the nozzle begins to generate thrust. Initially the pressure ratio is small and the flow at the exit is over-expanded and free boundary shock reflection is observed in the exhaust plume. With elapsed time the micro-valve continues to open and the pressure gradient across the nozzle increases as does thrust production. The size of the exhaust plume increases in tandem. As the micro-valve opens to its maximum position the flow transitions from over-expanded through perfectly-expanded and finally to under-expanded flow at steady-state; at this point a sizable expansion fan develops at the nozzle exit. This sequence is then repeated, in reverse order, during the shut-down process of the duty cycle.

Owing to viscous effects on the micro-scale, the use of inviscid theory in determining flow actuation and performance can lead to inaccurate impulse delivery predictions. Unfortunately, there has been little in the aerospace literature dealing with transient micronozzle operations, a fact primarily due to the large computational resources and effort required for the calculations. Here we describe results for a simulated firing of the NASA/GSFC hydrogen peroxide prototype with expander half-angles ranging from $10^\circ$–$50^\circ$ (Kujawa and Hitt, 2004; Louisos and Hitt, 2006a). Numerical simulations of transient flows have shown a finite time lag in thrust production and nozzle response occurs during the start-up sequence of the duty cycle. For the reduced pressure gradient across the nozzle during start-up, viscous effects dominate and the flow throughout the entire expander section is subsonic. As the pressure gradient increases with time, the flow locally attains supersonic velocities in a region extending downstream from the throat, but then decelerates to subsonic speeds by the nozzle exit. As the micro-valve continues to open and larger pressure gradients are established, the flow is able to overcome viscous forces and establish wide-spread supersonic conditions in the expander section. The lag in thrust production during start-up is most pronounced in the $10^\circ$ and $50^\circ$ expander half-angles owing to the fact that these geometries feature the largest subsonic layers.

In contrast, flow exhibits no lag in response to micro-valve closure during the shut-down sequence. Owing to the fact that viscous effects tend to reduce flow through frictional forces, the shut-down process is in fact facilitated by the existence of the subsonic layer. As the pressure ratio across the micronozzle is reduced during shut-down,
the subsonic layer grows into the bulk of the flow field and reduces the mass flow rate and thrust output. In this sense, viscous forces aid the shut-down sequence.

From a design standpoint, the net transient behaviour can be summarised by examining the total impulse delivered over one duty cycle for a single nozzle firing for various expander half-angles. The results are shown in Figure 10; also shown are the results from quasi-1D inviscid theory for comparison purposes. The total impulse from the simulations is less than that predicted by inviscid theory, which underscores the importance of accurately describing the joint viscous and geometric losses. The ‘optimal’ expansion half-angle for a linear micronozzle in the transient case is seen to be the same as for the steady-state operation (i.e., ~30°). This result here is coupled to the fact that the steady-state operation comprises roughly 18% of the duty cycle in the present model. Indeed, it is clear that optimisation of micronozzle geometry (angle) will be strongly case specific and strongly linked with the valve actuation characteristics.

**Figure 10** The total impulse generated by the micro-nozzle over one duty cycle normalized by quasi-1D inviscid theory. The micro-nozzle exhibits a maximum total impulse corresponding to the 30°.

### 4.4 The role of heat transfer

Micronozzles are typically fabricated into much larger, thermally-conducting substrates. In an operational setting, these substrates will be thermally linked with the remainder of the spacecraft and will experience major temperature variations over a single orbit (~90 min) due to alternating day/night conditions. It is thus expected that significant heat transfer is possible between the micronozzle and the substrate and, in turn, may impact the flow. As a first approximation, one may argue that the substrate can be regarded as a large thermal sink (or source) of constant temperature for the nozzle flow. This argument is based on a comparison of the relative thermal masses of the flow and a typical substrate, and consideration that a typical firing time for a microthruster is on the order of 1 s or less. As an example, a lumped capacitance analysis of the NASA/GSFC monopropellant microthruster suggests that only a 5% temperature increase would be realised within the substrate under a typical firing sequence involving a ‘cold’ initial state (Kujawa et al., 2003). Consistent with the assumption that the substrate
functions as an isothermal sink (source), we first consider performance under steady-state operation for varying isothermal boundary conditions. Isothermal nozzle wall temperatures ranging from 50 K to 1000 K have been examined to represent cases of a nanosat operating in day or night conditions. The alternative situation involving the transient heating of the substrate is considered in the following section.

4.4.1 Effects of nozzle wall temperature

To examine the effects of the wall boundary temperature, steady-state 2D numerical simulations of the NASA/GSFC hydrogen peroxide prototype operation have been performed for expander half-angles of 15°, 30° and 45° [Louisos and Hitt (2006b, 2007)]. Thrust production per unit micron of depth for steady 2D flow has been calculated for different isothermal wall temperatures and the results appear in Figure 11. In this figure, the thrust has been normalised by adiabatic quasi-1D theory and are also compared to the adiabatic simulations. It is observed that supersonic micronozzles with heat loss outperform comparable simulations with adiabatic nozzle walls.

Figure 11 Steady-state micronozzle performance with heat transfer through isothermal nozzle walls for a fixed Reynolds number of 800. A reduced wall temperature is used to model heat loss from the flow into the silicon substrate acting as a thermal sink. Note that the adiabatic results fall approximately on top of the 900 K isothermal wall values as indicated.

The observed effect of heat transfer can be readily explained from fundamental compressible flow theory (Rayleigh flow). It is known that removing heat from a supersonic flow acts to accelerate the flow (see Anderson, 2003). At steady-state, the bulk of the flow in the micronozzle expander is supersonic and thus heat transfer acts to further accelerate the supersonic flow at the nozzle exit. Heat extraction from the flow into the substrate increases performance from the subsonic layer point of view as well. For low nozzle wall temperatures, the local sonic velocity is diminished and hence the near-wall Mach number increases. This phenomena is the force driving the reduction in subsonic layer size for micronozzle flows with heat removal. The exact converse is true
for high-temperature walls, wherein an increase in the subsonic layer occurs and performance degrades.

In fact, with sufficient heat extraction from the flow, the subsonic layer can be reduced to the point where the competing effects of viscous forces and nozzle geometry cause the optimum expander half-angle to be shifted from \(30^\circ\) to a more typical traditional expander half-angle of \(15^\circ\). This is demonstrated in Figure 11 for isothermal wall temperatures less than \(~700\) K.

### 4.4.2 Transient heat transfer

As just demonstrated, heat transfer from the nozzle to its surroundings can have a significant impact on the supersonic flow within. From the design point of view, heat transfer affects thrust efficiency and can also **limit the burn time of a thruster**. The burn time of a thruster determines the total impulse bit available for a spacecraft propulsion maneuver. However, the heating of the microthruster structure due to the high-temperature supersonic flow in the nozzle imposes time limits on its operation, and consequently on the total impulse. The melting temperatures of the common materials used in MEMS-based thrusters, e.g., silicon and its compounds, are in the range of 1400–1700 K. The decomposition temperatures of about 2000 K are typical for solid propellants and such thrusters require short burn times or a cooling mechanism.

Indeed, the solution of the conjugate heat transfer problem will be an important part in future design optimisation process for supersonic micronozzles. The conjugate heat transfer for micronozzles is a coupled process of heat transfer between the gas and thruster walls, heat conduction in the solid and radiative heat transfer at the solid boundaries. The non-dimensional parameter that characterises the resistance of a material to heat conduction is the Biot number \(B_i = h_g L / k\) where \(h_g\) is the heat transfer coefficient between the gas and solid material, \(L\) is the characteristic length for heat conduction in the solid, which can be taken as the volume to surface ratio, \(L = V / A\), and \(k\) is the solid material thermal conductivity. Evidently, when the size of a thruster is scaled down, the Biot number decreases. Correlations for the heat transfer coefficient, \(h_g\), are available for turbulent and laminar flow regimes. For the conventional, large scale nozzles the turbulent correlation is used (Sutton and Ross, 2001):

\[
\text{Nu} = 0.026 \text{Re}^{0.8} \text{Pr}^{0.4}
\]

where \(\text{Nu} = h_g d / k_o\) is the local Nusselt number based on the nozzle diameter \(d\), \(\text{Re} = \rho V d / \mu\) is the local Reynolds number and \(\text{Pr} = \mu c_p / k_o\) is the Prandtl number. For the laminar flow, \(\text{Re} < 2300\), the following correlation applies (Ghajar and Tam, 1994):

\[
\text{Nu} = 1.24 \text{Re}^{1/3} \text{Pr}^{1/3} \left( \frac{d}{x} \right)^{1/3}
\]

where \(x\) is the distance from the nozzle inlet. Note, that in both turbulent and laminar regimes, the maximum heat transfer occurs at the nozzle throat.

For micronozzles, \(B_i \ll 1\) and the resistance to heat conduction in solid is much smaller than the resistance to convective heat transfer through the gas boundary layer. As a result, the temperature of the thruster solid material is nearly constant spatially but changes in time during a firing of the thruster.
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In Alexeenko et al. (2005, 2006) coupled gas flow and conjugate heat transfer simulations were applied for 2D and 3D modeling of a high-temperature decomposing solid propellant microthruster under development in NASA Glen Research Centre (Reed, 2003). The computational approach is based on the solution of the transient heat conduction problem in the silicon substrate coupled with the DSMC solution of the gas flow inside the micronozzle. The coupling between the material thermal response and fluid flow is carried out by using the DSMC calculated heat fluxes as the boundary condition in the heat conduction problem at the gas-solid interface. The wall temperature calculated in the heat conduction solution is in turn applied as a boundary condition in the gas flow simulation. The NASA Glen prototype micronozzle has a throat width of 300 µm, a depth of 600 µm and a length of 250 µm. The converging part of the nozzle has a half-angle of 30° and the inlet to throat area ratio of 10. The expansion half-angle of the diverging part is equal to 15° with an exit to throat area ratio of 5. Two cases of chamber pressure, 0.1 and 0.5 atm, were considered which correspond to the nominal Reynolds number at the throat equal to 35 and 175, respectively.

Rarefied gas flow modelling of thermal coupling between the micronozzle and the surrounding substrate shown that both the flow structure inside the micronozzle and performance parameters change significantly in time. The micronozzle flowfield structure is affected by the wall heat transfer as shown in Figure 12. The predicted thrust and mass flow rate of both 2D and 3D micronozzles decreases in time as the thickness of the boundary layer grows because of a hotter wall. For the lower stagnation pressure, \( p_0 = 0.1 \text{ atm} \), the final thrust value predicted by 3D simulations are 15% and 6% smaller than the initial values for Cases 1 (insulated outer wall) and 2 (cooled outer wall), respectively. The corresponding decrease of the thrust in the 2D nozzle is only 2–3%. For the 3D nozzle the initial value of the mass flow rate is 87% of that prescribed by the ideal nozzle theory (equation (9)). The final calculated values of the mass flow rate are 55% and 20% less than the initial values for Cases 1 and 2, respectively. Again, the change in mass flow with time is more pronounced in the 3D than the corresponding 2D model. For a larger stagnation pressure, \( p_0 = 0.5 \text{ atm} \), the initial value of the mass flow rate coefficient is 93% and it decreases to 68% and 81%, respectively, for Cases 1 and 2. Thus, the mass flow rate degradation is much more significant in the 3D. The main performance design implication of the conjugate heat transfer in micronozzles is the significant reduction in mass flow rates which was in all of the considered cases larger than the corresponding decrease in thrust.

5 Conclusions

Future generations of miniaturised spacecraft planned by NASA, ESA and other agencies will require unique propulsion systems capable of providing extremely low levels of thrust and impulse while concurrently satisfying stringent size and power constraints. While various micropropulsion schemes have been proposed, a key system component ubiquitous to all designs is the supersonic micronozzle. In this paper, we have demonstrated that the efficient design of supersonic nozzles on the micro-scale requires careful attention to effects not typically considered in macro-scale designs: viscous boundary layers; heat transfer; and flow rarefaction.

Viscous boundary layers within the supersonic expansion section can grow to occupy a substantial portion of the nozzle exit – in 2D planar and axisymmetric simulations, this
ranged from as little as 15% to as much as 100% depending on the mass flow rate (Reynolds number) and the thermophysical properties of the gas/mixture. Compensation for boundary layers by enlarging the expansion angle $\theta$ can likewise lead to performance reductions due to increased non-axial velocity components in the exit flow. A trade-off thus exists, and it follows that there will be some optimum nozzle expansion angle for which maximum performance is realised. Adiabatic nozzle simulations have indicated that maximum performance is obtained for nozzle expansion angles in the range of $25^\circ$–$30^\circ$; this is roughly twice the $15^\circ$ angle typically used in conical macro-scale thruster nozzles. The inherently 3D nature of actual MEMS-based micronozzles has been seen to reduce performance even further compared to 2D simulations.

**Figure 12** Conjugate heat transfer solution for nitrogen flow in a 3D microthruster at stagnation temperature of 2,000 K and stagnation pressure of 0.1 atm. The temporal variation of the gas and silicon substrate temperatures are shown in the thruster symmetry plane $Z = 0$. The heating of the substrate by the high-temperature gas flow changes both the flowfield structure inside the micronozzle and the thrust performance. The thrust value at time $t = 14.2$ s is 15% smaller than the initial value at time $t = 0$ s.

Heat transfer remains one of the more challenging considerations for conceptual micronozzle design since there are many unknowns with regards to the surrounding substrate material and its thermal state. Nonetheless, there are two general conclusions...
that can be drawn from heat transfer simulations. First, the combination of a large thermal mass and high thermal conductivity of a typical Si substrate allows for a simplifying lumped capacitance method to be used in many circumstances. Secondly, the overall effect of heat loss from the supersonic portion of the nozzle flow is beneficial to performance: the heat loss decreases the size of the subsonic layers near the walls and accelerates the bulk flow, giving rise to an increase in thrust production. It thus follows that the performance-optimising nozzle angle with heat loss will be smaller than the value predicted by adiabatic simulations.

Lastly, numerical simulations have shown that flow rarefaction effects on the nozzle walls give rise to near-wall subsonic layers whose thickness exceeds predictions from continuum analyses. The result of the increased subsonic portion of the nozzle flow is a diminished momentum flux at the nozzle exit and hence a reduction in thrust. DSMC simulations have suggested this effect can reduce nozzle efficiency by more than 20%. In fact, for flows with Reynolds numbers less than 100 at the throat the thrust performance of a converging/diverging nozzle is worse than that of a sonic orifice with no expander at all.

We close our discussion by mentioning two additional research areas in which future work is needed. The first involves multiphase flow (i.e., gas-liquid or gas-solids) in supersonic micronozzles. A gas-liquid scenario could arise with sufficiently high levels of heat loss through the nozzle walls resulting in gas condensation near the solid boundaries. This situation would most likely occur in the supersonic expansion section of the nozzle and the probable impact of condensation would be a reduction in thrust. The gas-solid scenario could arise with the use of solid propellants upstream of the nozzle. Here the incoming gas stream could contain residual micro-particles resulting from the ignition of the propellant. On the micro-scale, these particles could substantially alter the flow characteristics within the nozzle and dramatically reduce performance.

The second area for additional research involves design for plume-spacecraft interaction. As new micropropulsion concepts envision the use of micro-thruster arrays operating simultaneously to perform high-precision attitude control, an important design consideration is the backflow scattering of molecules that results from the interaction of multiple thruster plumes. Plume interactions impact spacecraft operation by altering the total thrust and the satellite lifetime due to increased mass, momentum and heat flux to the spacecraft surfaces. Depending on the configuration the total specific impulse of a thruster array can increase by as much as 16% compared to a single thruster (Ketsdever et al., 2004). However, the increase in thrust performance is metered by a significant increase in contaminant fluxes. Comprehensive spacecraft contamination studies for micropropulsion arrays will therefore require detailed analysis of plume/surface interactions based on rarefied gas dynamics methods, such as the DSMC approach.

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References


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Notes

1 Typically, this would imply concentrations between 85–90% with the remainder water.

2 Strictly speaking, one must also account for any mismatch between the nozzle exit pressure and the ambient pressure; however, this correction is usually small.

3 Several variants of the ‘conventional’ Burnett equations can now be found in the literature.