Numerical Investigation of Physical Processes in High-Temperature MEMS-based Nozzle Flows

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Abstract. Three-dimensional high-temperature flows in a MEMS-based micronozzle has been modeled using the DSMC method for Reynolds number at the throat from 30 to 440 and two different propellants. For these conditions, the gas flow and thrust performance are strongly influenced by surface effects, including friction and heat transfer losses. The calculated specific impulse is about 170 sec for Re=440 and about 120 sec for Re=43. In addition, the gas-surface interaction is the main mechanism for the change in vibrational energy of molecules in such flows. The calculated infrared spectra for the LAX112 propellant suggest that the infrared signal from such plumes can be detected and used to determine the influence of the cold wall boundary layer on the flow parameters at the nozzle exit.

INTRODUCTION

Currently, a number of MEMS-based micropropulsion concepts are being developed to meet the requirements of the future space missions. Fabrication of devices that use bi-propellant combustion and solid propellant (mono-propellant) decomposition was reported in Refs. [1, 2, 3]. In such devices, the obtained energetic gaseous mixture expands through a converging-diverging nozzle to create the thrust force. The gas flow in a MEMS-based nozzle is different from that in conventional macroscale nozzles due to a number of factors. First, the geometry of such nozzles is not axisymmetric as in their macroscale analogs. The MEMS-based nozzles usually have rectangular cross-sections due to the fabrication process. Next, the reduced scale influences the flow regime in these nozzles creating very low Reynolds number flows. In addition, the heat transfer losses can be extremely high if the wall temperature is much smaller than the stagnation temperature. Non-adiabatic and viscous flows do not lend themselves easily to a simple ideal nozzle theory treatment. These considerations make the numerical simulation of flows in micronozzle indispensable to assisting in design and experimental testing.

The 3-D flows in MEMS-based micronozzles have been studied numerically for cold gas and high-temperature thrusters. Both the kinetic (the direct simulation Monte Carlo method) and continuum (solution of Navier-Stokes equations) approaches were used. The results of the previous work[4] showed that the flow in high-aspect ratio nozzles is dominated by viscous losses for Re < 500. The comparison of the Navier-Stokes[5] and DSMC[6] modeling with experimental measurements[7] showed good agreement for mass flux but not for the measured and calculated thrust force. Such comparisons are complicated by the uncertainties in the experimental measurements due to the small scale of the force produced by such thrusters.

The main objective of this work is the study of the important physical processes that affect the flows in micro-scale nozzles. The influence of flow Reynolds number, internal energy relaxation, and gas-surface interactions are important components of a physical model to describe such flows. Models chosen for these processes must be suitable for use in numerical simulations. The DSMC method is used in all the flow calculations presented here. The internal energy of the gas is a small fraction of the total gas energy, hence internal energy exchange mechanisms may not significantly affect nozzle performance. However, specific gas vibrational states may be used to provide a diagnostic of the nature of the flow and in particular may elucidate the relative importance of gas-surface interactions. Such a concept will be evaluated here. In addition, the nozzle flow will be modeled for Reynolds numbers from 30 to 400 for two potential propellants and nozzle performance will be discussed.
FLOW CONDITIONS AND NUMERICAL METHOD

The geometric configuration of the micronozzle studied in this work corresponds to the microthruster design proposed by NASA Glenn researchers[3]. A single microthruster has a throat width of 300 \( \mu m \) and a depth of 600 \( \mu m \). The converging part of the nozzle has a half-angle of 30 deg and the expansion half-angle of the diverging part is equal to 15 deg with an exit to throat area ratio of 5. A schematic of the microthruster modeled here and axis notations used henceforth are shown in Fig. 1. The flow in such a microthruster is modeled for two different propellants: a decomposing solid propellant and a bi-propellant mixture. The first propellant is a solid compound 3,6-Diamino-1,2,4,5-tetrazine 1,4 dioxide (C_{2}H_{4}N_{6}O_{2}), known as LAX112. The main decomposition products of LAX112 propellant are nitrogen - 43 \%, carbon monoxide - 28.4 \% and hydrogen - 28.6 \%. Second, the products of hydrogen-air combustion at constant pressure and a stoichiometric fuel-to-oxidizer ratio were considered. The mole fractions of the major species are: N\(_{2}\) - 66 \%, H\(_{2}\)O - 32.5 \% and H\(_{2}\) - 1.5 \%. The flow conditions at the throat for two chamber pressures 0.1 and 1 atm are given in Table 2. Because the flow residence time is small, chemical reactions can be neglected. The Reynolds number is based on the throat width of 300 \( \mu m \) and the viscosity coefficient is calculated using Wilke’s rule for mixtures.

The DSMC method [8] has been applied in this work to obtain numerical solutions for low Reynolds number micronozzle flows. The DSMC-based software SMILE [9] is used for all computations. The code uses the majorant frequency scheme [10] of the DSMC method for collisional relaxation. The variable soft sphere model is used as the intermolecular potential. The discrete internal energy model was used in the calculations. The energy transfer between the translational, rotational, and vibrational modes was conducted according to the Larsen-Borgnakke model. Except for the H\(_{2}\)O molecules, temperature dependent rotational and vibrational collision numbers \( Z_r \) and \( Z_v \) were used, with the relaxation rates determined from Refs. [11, 12]. For the collisions between H\(_{2}\)O molecules, constant \( Z_r = 10 \) and \( Z_v = 10 \) were assumed. Constant \( Z_r = 10 \) and \( Z_v = 250 \) were used for the collisions between water molecules and other species. The Maxwell model with full momentum and energy accommodation is used for the gas-surface interaction. The wall temperature in such micronozzles is lower than the flow stagnation temperature (on the order of 2000 K) and an estimated value 600 C (872 K) is used in the calculations. The computational domain included the converging and diverging part of the micronozzle. The inlet to throat area ratio was 2. The conditions at the nozzle inlet were calculated using ideal nozzle theory. The vacuum boundary condition was used at the outflow boundary for a single micronozzle calculation. The linear cell size of the background collision grid was 10 \( \mu m \) for the \( p_0 = 1 \) atm case and 1 \( \mu m \) for \( p_0 = 1 \) atm, which is approximately equal to the throat mean free path. The average total number of molecules in the computational domain for the \( p_0 = 1 \) atm calculations was 25 million. The total time for the simulation in the \( p_0 = 1.0 \) atm case was 36 hours using 64 Pentium III 933 MHz processors.

RESULTS AND DISCUSSION

Flow structure

Let us first examine how the flowfield structure in the micronozzle changes for the two Reynolds number cases Re=44 and 443. These two cases correspond to the LAX112 propellant and stagnation pressures of \( p_0 = 0.1 \) and 1 atm, respectively. The flowfield contours are plotted in Figs. 2-6 for the two symmetry planes: Z=0 (bottom) and Y=0 plane (top). A significant boundary layer is observed in Figs. 2 and 3 for both Reynolds numbers with the thickness increasing for the more rarefied flow. In addition, for the lower Reynolds number case the boundary layer merges and there is no distinct inviscid core flow. The X-component of velocity along X-axis (nozzle centerline) is plotted in Fig. 4. In this figure X=0.26 mm corresponds to the nozzle throat and X=2.5 mm to the nozzle exit. For the lower Reynolds number case, the maximum velocity inside the nozzle occurs at one-third of the nozzle length. The translational temperature contours for the two Reynolds numbers are compared in Figs. 5 and 6. Although the inlet temperatures are equal for the two different stagnation pressures, the temperature in the diverging part of the nozzle is higher for the lower Reynolds number due to viscous dissipation.
Thermal non-equilibrium and viscous effects

For temperatures on the order of 1,000-2,000 K, translational-vibrational energy exchange is much slower than that between translational and rotational modes. This can lead to thermal non-equilibrium between different energy modes in nozzle flows. This is illustrated in the following two figures. The vibrational temperature profiles along the X-axis for each species of the LAX112 propellant mixture at $p_0 = 0.1$ atm are shown in Fig. 7. The vibrational temperature inside the nozzle is higher than the translational and rotational temperatures, plotted in Fig. 8. Though the vibrational temperature decreases with increasing distance along the X-axis, the decrease is due to collisions of gas molecules with the cold wall ($T_w = 872$ K) and not due to intermolecular collisions. The rate of vibrational energy exchange is slow ($Z_v \approx 10^6 - 10^8$) at these temperatures and the residence time ($\approx 10^3$ collision times) in the nozzle flow is much smaller than the characteristic vibrational relaxation time. The fact that the vibrational temperature decreases due to the gas-surface interaction is validated by the comparison of the mixture vibrational temperature profiles at two different pressures (Fig. 9). At higher pressure the vibrational energy exchange due to intermolecular collisions would be faster and vibrational temperature would be lower. Fig. 9 shows an opposite behavior: the vibrational temperature for $p_0 = 1$ atm case flow is higher than that for $p_0 = 0.1$ atm. This is due to the fact that at the lower pressure the gas-surface interaction effects are more pronounced. The calculation with a zero accommodation coefficient for vibrational energy showed that the vibrational temperature stayed constant and the vibrational energy exchange due to intermolecular collisions is negligible in this flow. For the full accommodation of vibrational energy, one can calculate the fraction of molecules that collided with the wall for a diatomic species as:

$$\omega = \frac{\exp(\theta_v/T_w) - 1}{\exp(\theta_v/T_i) - 1} \exp(\theta_i/T_w)$$

where $\theta_v = \theta_i / \log(1 + k \theta_v / \bar{E}_{vib})$, $T_i$ is the inlet temperature, $\bar{E}_{vib}$ is the average vibrational energy. Figure 10 shows the distribution of the fraction of molecules that collided with the wall for $N_2$ (top) and $H_2$ (bottom) for $Re=43$. Thus, on the X-axis and exit location about 54 % of nitrogen and 96 % of hydrogen molecules collided with the wall. Therefore, the change in vibrational temperature in low Reynolds number micronozzle flow is determined by the gas-wall interaction. The degree of the impact of wall and viscous effects can be estimated experimentally from the analysis of the spectroscopic measurement of the jet in the infrared region.

Infrared radiation of microthruster plumes

Carbon monoxide is a significant fraction of the LAX propellant decomposition products. To validate the simulations we consider whether the CO vibrational temperature could be estimated by Infrared (IR) spectroscopy. Although such experiments have not been performed on microthrusters, we can use the simulation results to calculate the well known vibrational spectra of the CO fundamental and first overtone to provide estimates of the predicted signal strength. The NEQAIR-IR radiation model of Laux et al.[14], an accurate line-by-line spectroscopic model, will be used. The NEQAIR model is sufficiently general that spectra may be calculated for gases that are in thermal nonequilibrium, i.e., one may assume that there are different translational, rotational, and vibrational temperatures. In addition, the NEQAIR computational tool carries out the complete wavelength dependent radiative transport calculation using a Voight profile, the most general line shape. We evaluate two possible locations where spectra might be observed, at the nozzle exit and 1 mm downstream of the nozzle exit. Figures 11-13 show profiles of the CO number density and translational and vibrational temperatures at the nozzle exit and 1 mm downstream of the nozzle exit. The CO number density profiles for the 0.1 atm pressure case are approximately one order of magnitude lower than those shown in Fig. 11. In all cases the profiles are taken in $Z=0$ plane from the outer boundary of the computational domain ($Y=1.5$ mm) to the to the x-axis.

To calculate the radiation that would be observed by a detector located in the vicinity of the outer edge of the plume, the temperature and CO number density profiles are reflected about the x-axis. The full temperature and CO number density profiles are then used in the NEQAIR-IR model to calculate spectra which are shown in Figs. 14 and 15. Consistent with Figs. 11-13, the spectral magnitude is larger at the exit than further downstream for both pressures and also scales with chamber pressure. A comparison of the exit spectra at 1 atm with a spectra calculated with the same conditions, but calculated as optically thin, indicated that the spectra shown in Fig. 14 is approximately 20 % optically thick in the wavelength region of the fundamental peak. Spectra computed 1 mm downstream of the nozzle, at both pressures, exhibit a different shape from the spectra at the exit. The spectral structure is sensitive to the gas rotational
and vibrational temperatures. This difference is due to the drop in translational temperature, which is assumed to be equilibrated with rotational temperature, as the gas expands. In contrast, the vibrational temperature profile changes only by approximately 100 K.

The predicted signal levels are sufficiently adequate to measure the spectra, if care is taken to minimize the noise background. A simpler measurement may also reveal information about the microthruster flow. If two radiometers are used to cover the fundamental and first overtone transition peaks, then the ratio of their signals may also provide a diagnostic. Table 2 shows the ratio of the predicted NEQAIR radiation for the fundamental to the first overtone, integrated over the individual peaks. Ratios are given for the two viewing locations and two chamber pressure cases as well as for a hypothetical situation where the vibrational temperature at the throat of $T_{\text{vib}}=1,720$ was assumed frozen even as the flow expanded. Such a situation might occur if the assumption of diffuse scattering of CO molecules with the cooler wall were incorrect.

Let us first consider the ratios obtained using the flowfield predictions in NEQAIR. The ratio is more sensitive to the chamber pressure, rather than either of the two locations. The ratio of the two peaks is approximately 40 for the 1 atm pressure case, regardless of whether it is taken at the exit or 1mm downstream. Similarly, the ratio for the 0.1 atm pressure cases are both approximately a factor of two higher. Now let us consider a second comparison of each case with the assumption of a fixed vibrational temperature. For both locations, the effect of holding the vibrational temperature constant on the ratio is small for a chamber pressure of 1.0 atm. However, for the lower pressure case of 0.1 atm the ratio would be reduced by approximately a factor of two for both locations. Since the boundary layer is larger in this case, the need to verify the gas-wall interaction is crucial. The sensitivity of the peak ratio to the calculated vibrational temperature spatial distribution could provide a useful, non-intrusive flow diagnostic.

**Microthruster performance for different propellants**

Now we compare the calculated performance characteristics for the two propellants and two stagnation pressures. The momentum flux in X-direction normalized by its throat value is given in Fig. 16. The plot shows that at $Re<400$ the micronozzle is less efficient because the momentum flux in the diverging section decreases compared to the value at the throat due to heat transfer and friction losses. The calculated discharge coefficient, thrust force, and specific impulse are listed in Table 3. The discharge coefficient is lower for the hydrogen-air propellant by approximately 5 % for both pressures. This is due to the difference in the viscosity coefficient of the two mixtures ($\nu = 0.0066 \text{ m}^2/\text{sec}$ for LAX112, $\nu = 0.0088 \text{ m}^2/\text{sec}$ for hydrogen-air propellant at the throat for the $p_0 = 0.1 \text{ atm}$ case). For both propellants, the specific impulse for $p_0 = 0.1 \text{ atm}$ case is about 30 % smaller than for $p_0 = 1.0 \text{ atm}$ due to larger friction and heat transfer losses.

**CONCLUSIONS**

Numerical modeling of three-dimensional flow in MEMS-based nozzles for Reynolds numbers from 30 to 443 has been conducted using the DSMC method. Two potential propellant options have been compared, the solid propellant LAX112 and a hydrogen-air propellant. The viscous and heat transfer losses are significant in this flow regime for both propellants with the specific impulse for $p_0 = 0.1 \text{ atm}$ case about 30 % smaller than for $p_0 = 1.0 \text{ atm}$.

The infrared radiation signatures have been calculated for the LAX112 propellant case at stagnation pressures $p_0 = 0.1$ and 1 atm. The radiation signal was found to be detectable for the considered flow conditions. We suggest to use the infrared radiation measurements to diagnose the influence of the boundary layer in such flows. Namely, the ratio of radiation intensity of the two CO peaks depends strongly on the vibrational temperature at the nozzle exit. The vibrational temperature is unaffected by the influence of the cold wall in the higher Reynolds number case ($Re=443$), but is sufficiently decreased due to the interaction with a cold wall at lower pressures ($Re=43$).

**ACKNOWLEDGMENT**

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TABLE 1. Flow conditions at the throat, LAX propellant

<table>
<thead>
<tr>
<th>Propellant</th>
<th>$p_0$ (atm)</th>
<th>$n_t$ (mol/m$^3$)</th>
<th>$T_t$ (K)</th>
<th>$U_t$ (m/sec)</th>
<th>Re</th>
</tr>
</thead>
<tbody>
<tr>
<td>LAX 1.</td>
<td>1.0</td>
<td>$2.36\times10^{24}$</td>
<td>1722</td>
<td>972.7</td>
<td>443</td>
</tr>
<tr>
<td>LAX 0.1</td>
<td>0.1</td>
<td>$2.37\times10^{23}$</td>
<td>1721</td>
<td>973</td>
<td>44.3</td>
</tr>
<tr>
<td>H$_2$-air 1.</td>
<td>1.0</td>
<td>$1.9\times10^{24}$</td>
<td>2078</td>
<td>950</td>
<td>300</td>
</tr>
<tr>
<td>H$_2$-air 0.1</td>
<td>0.1</td>
<td>$2.0\times10^{23}$</td>
<td>1996</td>
<td>932</td>
<td>32</td>
</tr>
</tbody>
</table>

TABLE 2. Ratios of peak integrated radiation intensity for the fundamental to the first overtone.

<table>
<thead>
<tr>
<th>Condition</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>exit, 1 atm</td>
<td>37.3</td>
</tr>
<tr>
<td>exit, 1 atm, $T_{ vib}=1,720$</td>
<td>33.7</td>
</tr>
<tr>
<td>exit, 0.1 atm</td>
<td>89.0</td>
</tr>
<tr>
<td>exit, 0.1 atm, $T_{ vib}=1,720$</td>
<td>40.0</td>
</tr>
<tr>
<td>1mm, 1 atm</td>
<td>41.1</td>
</tr>
<tr>
<td>1mm, 1 atm, $T_{ vib}=1,720$</td>
<td>37.4</td>
</tr>
<tr>
<td>1mm, 0.1 atm</td>
<td>100.8</td>
</tr>
<tr>
<td>1mm, 0.1 atm, $T_{ vib}=1,720$</td>
<td>40.8</td>
</tr>
</tbody>
</table>

TABLE 3. Calculated micronozzle performance

<table>
<thead>
<tr>
<th>Propellant</th>
<th>$p_0$, atm</th>
<th>$c_d$, %</th>
<th>$T$, mN</th>
<th>$I_{sp}$, sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>LAX112</td>
<td>0.1</td>
<td>91.7</td>
<td>1.53</td>
<td>124.6</td>
</tr>
<tr>
<td>LAX112</td>
<td>1.0</td>
<td>96.8</td>
<td>22.1</td>
<td>169.2</td>
</tr>
<tr>
<td>H$_2$-air</td>
<td>0.1</td>
<td>86.4</td>
<td>1.37</td>
<td>117.4</td>
</tr>
<tr>
<td>H$_2$-air</td>
<td>1.0</td>
<td>93.4</td>
<td>21.1</td>
<td>167.8</td>
</tr>
</tbody>
</table>

FIGURE 1. Schematic of the microthruster.

FIGURE 2. X-component of velocity contours for $p_0 = 0.1$ atm, LAX112. Y=0 - top (area shown is 3.3 mm x 0.4 mm), Z=0-bottom (area shown is 3.3 mm x 1.5 mm).

FIGURE 3. X-component of velocity contours for $p_0 = 1.0$ atm, LAX112. Y=0 - top (area shown is 3.3 mm x 0.4 mm), Z=0-bottom (area shown is 3.3 mm x 1.5 mm).

FIGURE 4. X-component of velocity profile along x-axis, LAX112.
FIGURE 5. Translational temperature contours for $p_0 = 0.1$ atm, LAX112. Y=0 - top (area shown is 3.3 mm x 0.4 mm), Z=0-bottom (area shown is 3.3 mm x 1.5 mm).

FIGURE 6. Translational temperature contours for $p_0 = 1.0$ atm, LAX112. Y=0 - top (area shown is 3.3 mm x 0.4 mm), Z=0-bottom (area shown is 3.3 mm x 1.5 mm).

FIGURE 7. Vibrational temperature along the x-axis for $p_0 = 0.1$ atm, LAX112.

FIGURE 8. Translational and rotational temperature along the x-axis for $p_0 = 0.1$ atm, LAX112.

FIGURE 9. Vibrational temperature along the x-axis for $p_0 = 0.1$ and 1.0 atm, LAX112.

FIGURE 10. Fraction of molecules collided with the wall for $p_0 = 0.1$, CO (top) and H$_2$ (bottom).
FIGURE 11. Profiles of CO number density for the 1.0 atm pressure case, LAX112 propellant.

FIGURE 12. Profiles of temperatures for the 1.0 atm pressure case, LAX112 propellant.

FIGURE 13. Profiles of temperatures for the 0.1 atm pressure case, LAX112 propellant.

FIGURE 14. Calculated IR spectra of CO fundamental and first overtone for a chamber pressure of 1 atm at the exit and 1 mm downstream from the exit.

FIGURE 15. Calculated IR spectra of CO fundamental and first overtone for a chamber pressure of 0.1 atm at the exit and 1 mm downstream from the exit.

FIGURE 16. Momentum flux in x-direction normalized by its value at the throat.
REFERENCES