Supplementary Material

1 0D ELECTRON ENERGY EQUATIONS

Electron temperature is related to electron energy u_e as

$$T_{e,i} = \frac{2u_{e,i}}{3\sum_{s+} n_{s+,i}} \tag{S1}$$

$$T_{e,a} = \frac{2u_{e,a}}{3\sum_{s+} n_{s+,a}} \tag{S2}$$

In the ionization and acceleration stages control volumes, we express electron energy conservation as

$$\frac{du_{e,i}}{dt} = \frac{5}{2}\left(\frac{\Gamma_{e,a\to i}T_{e,a} - \Gamma_{e,i\to an}T_{e,i}}{V_i}\right) + \frac{\int n_e \mathbf{v_e}\cdot\nabla\mathbf{\Phi}\,\mathrm{d}V_i}{V_i} - \beta\sum_j \nu_{e,j}k_j(T_{e,i})n_{j,i}n_{e,i}\epsilon_j - \frac{S_{w,i}-S_{an}}{S_{w,i}}\sum_{s+}\frac{(1-\alpha_{s+,i})n_{s+,i}}{\tau_{s+,i}}\left[\frac{2T_{e,i}}{1-\gamma_s(T_{e,i})}+\Phi_{s,i}\right] \tag{S3}$$

$$\frac{du_{e,a}}{dt} = \frac{5}{2}\left(\frac{\Gamma_{e,cat\to a}T_{e,tr} - \Gamma_{e,a\to i}T_{e,a} - \Gamma_{e,a\to ie}T_{e,a}}{V_a}\right) + \frac{\int n_e \mathbf{v_e}\cdot\nabla\mathbf{\Phi}\,\mathrm{d}V_a}{V_a} - \beta\sum_j \nu_{e,j}k_j(T_{e,a})n_{j,a}n_{e,i}\epsilon_j - \frac{S_{w,a}-S_{ie}}{S_{w,a}}\sum_{s+}\frac{(1-\alpha_{s+,a})n_{s+,a}}{\tau_{s+,a}}\left[\frac{2T_{e,a}}{1-\gamma_s(T_{e,a})}+\Phi_{s,a}\right] \tag{S4}$$

where the four terms in the right-hand side of the Equation S3 and S4 respectively represents electron energy transport, electric field work, ionization losses, and energy losses at insulating walls. These equations contain two semi-empirical parameters: the mean energy cost per ionization event β and Bohm's anomalous diffusion coefficient α_B. β mainly accounts for excitation losses, having reported values of 3 for Hall thruster Xe discharges (1), and still to be calibrated on experimental data for atmospheric propellant. The electron trigger velocity $v_{e,tr}$ is computed from the 2D magnetic and potential fields solution data as

$$v_{e,tr} = \int_{A_{a,out}} \bar{\bar{\mu}}\cdot\nabla\phi\cdot\frac{\mathrm{d}A}{A_{a,out}} \tag{S5}$$

where $A_{a,out}$ is the outlet area of the acceleration stage control volume and $\bar{\bar{\mu}}$ is the electron mobility tensor.

The electron fluxes Γ_e appearing in the energy transport terms are defined as follow:

- the electrons emitted by the cathode which triggers the acceleration stage discharge

$$\Gamma_{e,cat\to a} = V_a\sum_{s+}\frac{\alpha_{s+,a}n_{s+,a}}{\tau_{s+,a}u_{s+,a}}v_{e,tr} \tag{S6}$$

- the electrons collected by the acceleration stage intermediate electrode

$$\Gamma_{e,a\to ie} = S_{ie}\sum_{s+}\frac{V_a}{S_{w,a}}\frac{(1-\alpha_{s+,a})n_{s+,a}v_{e,th}}{\tau_{s+,a}}\sqrt{\frac{M_s}{2\pi m_e}}e^{-\frac{\Phi_{sh}}{T_{e,a}}} \tag{S7}$$

- the electrons collected by the ionization stage anode

$$\Gamma_{e,i\to an} = S_{an}\sum_{s+}\frac{V_i}{S_{w,i}}\frac{(1-\alpha_{s+,a})n_{s+,i}v_{e,th}}{\tau_{s+,i}}\sqrt{\frac{M_s}{2\pi m_e}}e^{-\frac{\Phi_{sh}}{T_{e,i}}} \tag{S8}$$

- the electrons flowing from the acceleration to the ionization stage control volume

$$\Gamma_{e,a\to i} = \Gamma_{e,cat\to a} - \Gamma_{e,a\to ie} + V_a\sum_{s+}\frac{\alpha_{s+,a}n_{s+,a}}{\tau_{s+,a}} - V_i\sum_{s+}\frac{\alpha_{s+,i}n_{s+,i}}{\tau_{s+,i}} \tag{S9}$$

where S_{an} and S_{ie} are respectively the ionization stage anode and intermediate electrode area, $T_{e,tr}$ is the temperature of the electrons emitted by the cathode (usually in the order of a few eV and having a small impact on the electron temperature solution), and Φ_{sh} is the plasma sheath potential in front of the two thruster electrodes (namely, the ionization stage anode and the acceleration stage intermediate electrode). At each time step, the sheath potential Φ_{sh} is computed by imposing the electronic current collected by the thruster electrodes to be equal to the total electronic current emitted by the cathode.

The electron fluxes defined in Equation S6 to S9 allow to estimate the electric field work in the two stage control volumes:

$$\int_{V_i} n_e\mathbf{v_e}\cdot\nabla\phi\,\mathrm{d}V = \int_{V_i}\nabla\cdot(\phi n_e\mathbf{v_e})\,\mathrm{d}V - \int_{V_i}\phi\nabla\cdot(n_e\mathbf{v_e})\,\mathrm{d}V = \Gamma_{e,i\to an}\phi_{an} - \Gamma_{e,a\to i}\phi_{a,in} - (\Gamma_{i,a\to an} - \Gamma_{e,a\to i})\phi_i \tag{S10}$$

$$\int_{V_a} n_e\mathbf{v_e}\cdot\nabla\phi\,\mathrm{d}V = \Gamma_{e,a\to i}\phi_{a,in} - \Gamma_{e,cat\to a}\phi_{a,out} - (\Gamma_{e,a\to i} - \Gamma_{e,cat\to a})\phi_a \tag{S11}$$

where

$$\phi_i = \int_{V_i}\phi\mathrm{d}V/V_i \tag{S12}$$

$$\phi_{a,in} = \int_{A_{a,in}}\phi\mathrm{d}A/A_{a,in} \tag{S13}$$

$$\phi_a = \int_{V_a}\phi\mathrm{d}/V_a \tag{S14}$$

$$\phi_{a,out} = \int_{A_{a,out}}\phi\mathrm{d}A/A_{a,out} \tag{S15}$$

are computed from the 2D potential solver solution data. In Equation S3 and S4, the energy loss at insulating walls are estimated according to the formulation presented in (2), where the wall sheath potential Φ_s is expressed as

$$\phi_s = T_e \ln\left[\sqrt{\frac{M_s}{2\pi m_e}}(1-\gamma_s(T_e))\right] \tag{S16}$$

and the semi-empirical relation for BN secondary electron emission derived in (3) is used for $\gamma_s(T_e)$:

$$\begin{aligned}\gamma_s = \sqrt{T_e/0.35} \quad if \quad \gamma_s < 1-8.3\sqrt{m_e/M_s}\\ \gamma_s = 1-8.3\sqrt{m_e/M_s} \quad if \quad \gamma_s \geq 1-8.3\sqrt{m_e/M_s}\end{aligned} \tag{S17}$$

2 NEUTRAL MONTE CARLO PERFORMANCE AND VALIDATION

We evaluated code performance for a sample intake design having an aspect ratio $d_1 = 9$ and an area ratio $d_2 = 7.5$. Uncertainty evaluation of the resulting transmission probability, mean residence time, compression ratio and computational time is reported in Table S1 for 1e2, 1e3, 1e4 and 1e5 simulated particles. Precision uncertainty is estimated by repeating each simulation 100 times and computing the confidence level as $CL_{99.7\%} = 3\sigma/\sqrt{N}$. All computations were performed on a 2.3GHz quad-core Intel i5 processor. Table S1 reports the average computational time per simulation, labelled as T_C.

N_2 Particles	$\alpha_{N_2,itk}$	$\tau_{N_2,i}$ [ms]	r_{N_2}	T_C [s]
$1e2$	0.2285 ± 0.0123	1.487 ± 0.111	222.0 ± 20.5	0.2472
$1e3$	0.2315 ± 0.0042	1.450 ± 0.028	218.8 ± 5.5	1.208
$1e5$	0.2301 ± 0.0012	1.451 ± 0.009	217.7 ± 1.7	10.44
$1e6$	0.2301 ± 0.0004	1.445 ± 0.003	216.8 ± 0.6	118.3

Table S1. Simulation Data for the Reference Intake Test Case.

Code accuracy for 1e5 simulated particles was validated against literature results of rarefied flow simulation implementing the CLL scattering kernel (4). Table S2 shows the output transmissions for conical ducts of different aspect ratio L/R and conical angle β as compared to the ones provided in (4). To perform the code validation, the thruster geometry was removed, the intake wall temperature set equal to inlet flow temperature and the collimated flow velocity u_∞ set equal to 0. The conical intake geometry parametrization provided in this work is related to Sharipov conical duct parametrization as $d_1 = L/R$ and $d_2 = [1/(1 + L/R\tan(\beta))]^2$.

	Sharipov				Neutral Monte Carlo			
L/R	β =0°	15°	30°	45°	β =0°	15°	30°	45°
0.1	0.9556	0.9763	0.9889	0.9958	0.9575	0.9794	0.9868	0.9994
0.2	0.9155	0.9557	0.9799	0.9927	0.9199	0.9597	0.9763	0.9890
0.5	0.8155	0.9083	0.9615	0.9874	0.8137	0.9036	0.9649	0.9888
1	0.6948	0.8587	0.9459	0.9840	0.6913	0.8549	0.9479	0.9849
2	0.5436	0.8087	0.9342	0.9821	0.5450	0.8105	0.9357	0.9830
5	0.3385	0.7629	0.9273	0.9813	0.3387	0.7651	0.9279	0.9813
10	0.2117	0.7469	0.9258	0.9813	0.2090	0.7497	0.9251	0.9805
20	0.1224	0.7405	0.9255	0.9813	0.1222	0.7383	0.9244	0.9821

Table S2. Neutral Monte Carlo Simulation of conical ducts as compared to literature results by Sharipov (4) for $\sigma_n = 1$ and $\sigma_t = 0.9$.

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