Informing the Design of Pure-ion Electrospray Thrusters via Simulation of the Leaky-Dielectric Model with Charge Evaporation

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Electrosprays operating in the pure-ion regime (PIR) are of particular interest to space propulsion due to its ability to produce high specific impulse and efficient electrical-to-kinetic energy transformation, concurrently with its simplicity and compactness. Unlike electrospray emitters operating in the droplet mode, pure-ion emission using ionic liquids (IL) is known to be highly dependent on the meniscus configuration and the upstream conditions of the source, and consequently permissible under specific circumstances, related to its stability. This has conferred pure-ion sources with increased difficulty in controlling and predicting fundamental beam characteristics such as current emitted, while also making it hard to establish the conditions that need to be met by the device structure to support adequate ion emission. Therefore, leading the design of tips to rely on empirical trends, generically based on trial and error.

In this paper, a combination of two computational frameworks are proposed, that aim to push the transition from the current empirical design mindset to a quantitative physics-based model. The first framework utilizes Darcy’s law to calculate a hydraulic impedance of a given emitter tip design. The second framework combines the impedance of an emitter tip, and the physical properties of an IL to compute useful metrics for propulsion (e.g, current emitted, meniscus stability, and physical fields’ distributions). It is built on the foundation of past research on the Taylor-Melcher multi-physics leaky-dielectric model accounting for charge evaporation.

Preliminary results indicate that meniscuses operating in the PIR are small (∼1 µm), and need a minimum value of hydraulic impedance to operate in a stable regime.

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Nomenclature of physical constants

\(k_B\) = Boltzmann constant, \(\text{m}^2 \text{kg s}^{-2} \text{K}^{-1}\)
\(\Delta G\) = solvation energy, \(\text{J}\)
\(e\) = elementary electron charge, \(\text{C}\)
\(\varepsilon_0\) = vacuum electric permittivity, \(\text{F m}^{-1}\)
\(\varepsilon_r\) = relative dielectric permittivity
\(h\) = Planck constant, \(\text{m}^2 \text{kg s}^{-2}\)
\(\gamma\) = surface tension, \(\text{N m}^{-1}\)
\(T_0\) = reference temperature, \(\text{K}\)
\(k_0\) = fluid conductivity at the reference temperature, \(\text{S}\)
\(k'\) = linear fluid conductivity sensitivity to temperature variations, \(\text{S K}^{-1}\)
\(\mu_0\) = dynamic viscosity at the reference temperature, \(\text{m}^2 \text{s}^{-1}\)
\(\rho\) = density, \(\text{m}^3\)
\(q\) = average emitted ion charge, \(\text{C}\)
\(m\) = average emitted ion mass, \(\text{kg}\)
\(Z_{int}\) = internal impedance of emitter tip, \(\text{kg m}^{-4} \text{s}^{-1}\)
\(Z_{ext}\) = external impedance of emitter tip, \(\text{kg m}^{-4} \text{s}^{-1}\)
\(Z_{bulk}\) = internal impedance of emitter tip base substrate, \(\text{kg m}^{-4} \text{s}^{-1}\)
\(Z_{tot}\) = total impedance of unit cell, \(\text{kg m}^{-4} \text{s}^{-1}\)
\(Q\) = volumetric flow rate, \(\text{m}^3 \text{s}^{-1}\)
\(\kappa\) = permeability, \(\text{m}^2\)
\(D_{eff}\) = particle size, \(\text{m}\)
\(R_c\) = radius of curvature, \(\text{m}\)
\(D_p\) = pore size, \(\text{m}\)
\(D_g\) = groove size, \(\text{m}\)
\(\phi_p\) = open volume fraction
\(t\) = thickness of base substrate, \(\text{m}\)
\(h\) = height of emitter tip, \(\text{m}\)
\(A\) = cross-sectional area, \(\text{m}^2\)
\(\alpha\) = half-cone angle, \(\circ\)
\(I_e m\) = emitted current, \(\text{A}\)
I. Introduction

The demand for high efficiency, compact, and scalable propulsion devices have impulsed electrospray technology to the reference of nanosatellite propulsion systems. Electrospray or colloidal propulsion systems operate by accelerating matter extracted from a conductive liquid surface using high electric fields. The driving electrostatic force is enhanced by a sharp geometrical feature, such as a needle, at the tip of which a cone-like liquid meniscus forms.

Geoffrey Taylor demonstrated that the interface approaches a perfect conical geometry with a half-angle of $\theta_T = 49.29^\circ$ when differences in hydrostatic pressure between the liquid and the external dielectric medium are neglected, and no space charge is considered. This universal angle withstands experimentally for many cases to a very good approximation, despite the aforementioned assumptions. The singular behavior of the electric field created near the apex of the cone $\left( E_n \propto \frac{1}{r} \right)$ causes it to deform in a thin jet that breaks into droplets downstream as a result of capillary Rayleigh instability. These droplets are accelerated to create thrust in traditional electrospray thrusters.

When the flow rate is reduced while maintaining a high liquid conductivity, the maximum electric field along the cone-jet surface starts to increase. When this field reaches a critical value $E^*$, on the order of $1 \sim 2 \frac{V}{nm}$, a process known as field evaporation begins to release low-solvation ions from the meniscus surface in parallel to droplets.

For limited types of fluids such as liquid metals and ionic liquids, if the flow rate is further reduced, i.e., by increasing the hydraulic impedance, the jet becomes unstable until the point where droplet emission is no longer sustained and only ions are emitted from a stressed, closed-surface of the liquid. This current emission mode is known as the Pure Ion Regime (PIR). Empirically it has been shown that a hydraulic impedance of at least $\sim 1.5 \cdot 10^{17}$ kg m$^{-4}$ s$^{-1}$ is required to produce PIR. The mass-to-charge ratio ($\frac{q}{m}$) from PIR is very appealing for nanosatellite propulsion due to its ability to produce high specific impulses and efficiencies.

Ionic liquids are a type of room temperature molten salts that have virtually zero vapor pressure, in virtue of the coulombic intermolecular forces. Unlike liquid metal ion sources (LMIS), ionic liquid ion sources (ILIS) are of particular interest because of their tunability. Up to $10^{18}$ combinations of anion-cation pairs are reported to be feasible. This versatility gives access to a wide range of cation and anion pairs to optimize both the physical properties and the specific molecular chemistries for propulsion applications. For instance, emission of heavy ions is desired to maximize the thrust-to-power ratio $\left( \frac{F}{P} \propto \frac{1}{r} \right)$. Furthermore, IL-based propulsion devices can be operated as power-efficient systems; no energy spent on propellant liquefaction or ionization since molecular ions are readily extracted from the propellant bulk. Microthrusters based on ionic liquids can also produce both positive and negative ions. This is beneficial for spacecraft charging issues, as neutralization of the beam can be achieved by operating pairs of thrusters in opposite polarities.

Unlike LMIS, where space charge enhances the stability of the meniscus by shielding the effects of external electric perturbations, ILs space charge effects are negligible, which makes the quality of the source more susceptible to the specific properties of the working ionic liquid and emitter geometry.

Experimental difficulties of resolving properties like the PIR meniscus interface profile, fluid interaction with the tip and characteristics of internal creeping flow have hindered fundamental understanding of ILIS. Especially the role of key operating parameters such as the external electric field, the size of tip inlet pores or the hydraulic impedance of the feeding material in the total current emitted or meniscus stability. Furthermore, limited research has been conducted on the full characterization of the hydraulic impedances of porous electrospray emitters, specifically accounting for both the internal and external wetting.

For this reason, the design approaches of ILIS as propulsion devices have been predominantly empirically informed trial and error.

Two major attempts to model ILIS exist in the literature. Higuera modeled a small volumetrically-constrained ionic liquid drop under steady charge evaporation attached to a flat conducting plate. The equations were adapted from the Taylor-Melcher leaky dielectric model including charge evaporation. Coffman advanced Higuera’s model by removing the volumetric constraints and accounting for Ohmic heating effects. The works by Higuera and Coffman produced surface shapes that differ substantially from Taylor cones, where stability is found when feeding architectures favor high hydraulic impedances, small meniscus characteristic lengths and limited range of operating voltages.

In this paper, a computational framework building on Higuera and Coffman’s work to push the shift from the current empirical paradigm of ILIS design practices towards a rigorous quantitative physics-based
approach is presented. The two computational models presented: The first estimates the total hydraulic impedance for a given extractor geometry. The second one uses the aforementioned hydraulic impedance and other operational inputs to infer properties useful for propulsion, namely current emission or static stability of the meniscus. These properties can be used to inform important design parameters for ILIS in the PIR such as pore sizes, tip radius of curvature and conical tip semiangle.

II. Overview

Figure 1 illustrates an idealized version of an extractor tip array. The ionic liquid propellant can be considered to be situated in a reservoir at pressure $p_r$ below the extractor tip. The propellant flows through the porous substrate due to capillary action and forms a small meniscus at the apex of the tip. The propellant evaporates in a small region $r^*$ at the surface of the meniscus in the form of ions, which are accelerated through an extractor grid to create the thrust. The differential hydraulic impedance model calculates how much pressure drop the propellant experiences per unit flow rate $Q$ or current $I$ due to friction with the walls. This hydraulic impedance depends on the properties of the porous material and tip geometry. The Coffman model is centered at the apex of the tip and calculates the meniscus shape in static equilibrium associated with the aforementioned hydraulic impedance and external extracting potential.

III. Numerical methodology

A. Coffman model

1. Geometry Description

The simulated axisymmetric domain is shown in figure 2 and aims to reproduce the physics vicinity of the apex of the tip, where the meniscus forms. In this problem, a column of fluid of radius $r_0$ is considered that is attached to a downside conducting electrode ($\Gamma_D$) with the shape of a flat plate of radius $r_p$. For the sake of simplicity, the effects of tip curvature are ignored. The downstream electrode is biased with a potential difference $\Delta V = E_0 z_0$ with respect to a flat upstream electrode ($\Gamma_U$) at a distance $z_0$ so that an electric field exists in the region in-between. The fluid column ($\Omega_l$) can be understood as a tube connecting the vacuum open space between the two electrodes ($\Omega_v$) with the fluid reservoir at pressure $p_r$. This reservoir is not treated computationally. The fluid enters the computational domain at $\Gamma_I$, which is at a distance $z_p$ from the downstream electrode; as if it were the outlet of a fully developed pipe flow (Hagen-Poiseuille paraboloidal flow). It is accelerated through the vicinity of the emission region (close to the meniscus apex) and released to the external vacuum region in the form of evaporated ions. The same situation is considered as Coffman, where the liquid column contact line with the downside plate is fixed (pinned), while the contact angle of the meniscus interface $\Gamma_M$ with the downside electrode is free to adopt any value $\theta$. 

Figure 1: Simplified diagram of an array of tips with an emitting meniscus formed at the apex.
2. Characteristic orders of magnitude of pure-ion evaporation

Figure 2 also shows a diagram of the emission region in the vicinity of the meniscus tip. Iribarne and Thomson suggested that electrically-assisted charge emission in high conductivity fluids like ionic liquids can be modeled as an activated process:

\[ j_n^e = \frac{\sigma k_B T}{h} \exp \left( -\frac{E_a}{k_B T} \right) \]  \hspace{1cm} (1)

Where \( j_n^e = \langle \mathbf{j} \cdot \hat{n} \rangle \) is the local current density emitted at the surface of the meniscus, \( E_a = \Delta G - G (E_n^*) \) is the activation energy, \( T \) is the liquid temperature and \( \sigma \) is the surface charge on \( \Gamma_M \).

An image charge argument can be brought into consideration when analyzing the dependence of the meniscus surface. It can be shown that in this region, the ionic liquid meniscus behavior approaches that of a perfect dielectric fluid where \( E^* \) is the critical electric field from which the closed meniscus will start emitting charge is:

\[ E^* = 4\pi \varepsilon_0 (\Delta G)^2 \]  \hspace{1cm} (2)

For typical values of ionic liquids, this critical electric field is on the order of \( 10^9 \text{V/m} \).

If the emission region is modeled as a spherical cap and by neglecting any hydrodynamic pressure, the balance of stresses in the normal direction should be:

\[ \frac{1}{2} \varepsilon_0 E_n^{v2} - \frac{1}{2} \varepsilon_r E_n^r 2 = \frac{2\gamma}{r^2} \]  \hspace{1cm} (4)

Where \( r^* \) is the radius of this spherical cap and \( E_n^r \) is the internal local electric field perpendicular to the meniscus surface. It can be shown that in this region, the ionic liquid meniscus behavior approaches that of a perfect dielectric fluid where \( E_n^r \approx \frac{E_n^v}{\varepsilon_r} \). If the meniscus is emitting, it will adapt its surface shape so that \( E_n^v \sim E^* \). Using these two assumptions, the balance of stresses in equation 4 yields:

\[ \frac{1}{2} \varepsilon_0 E_n^{v2} \varepsilon_r - \frac{1}{\varepsilon_r} E_n^r = \frac{2\gamma}{r^*} \]  \hspace{1cm} (5)

For typical ionic liquids where \( \varepsilon \gg 1 \), the characteristic emission radius yields:

\[ r^* = \frac{4\gamma}{\varepsilon_0 E_n^{v2}} \]  \hspace{1cm} (6)

Where \( r^* \) is on the order of \( 10^{-8} \sim 10^{-10} \text{m} \).

The total current emitted can be stated as:

\[ I^* = j^* A = k E_n^r A = \frac{k E_n^r}{\varepsilon_r} 2\pi \left( r^* \right)^2 = \frac{32\pi k \gamma^2}{\varepsilon_0^2 \varepsilon_r E_n^{v2}} \]  \hspace{1cm} (7)

Where \( j^* \approx k E_n^r \approx \frac{k E_n^v}{\varepsilon_r} \) is the characteristic current density in the emission region, \( k \) is the electrical conductivity and \( A = 2\pi \left( r^* \right)^2 \) is the area of the spherical cap. For typical ionic liquids, \( I^* \) is on the order of 50 to 500 nA.

3. Model equations

The model of a statically-emitting free volume ionic liquid ion source involves electrohydrodynamic physics as well as energy transport phenomena. Table I shows the set of non-dimensional equations fulfilled in the bulk domains. Lengths have been non-dimensionalized by the contact line radius \( r_0 \left( \hat{r} = \frac{r}{r_0} \right) \), pressures and stresses by \( p_c = \frac{2 \gamma}{r_0} \left( \hat{p} = \frac{p}{p_c} \right) \), and electric fields by \( E_c = \sqrt{\frac{4\gamma}{\varepsilon_0 r_0}} \left( \hat{E} = \frac{E}{E_c} \right) \), surface charge by \( \sigma_c = \varepsilon_0 E_c \)
Figure 2: Computational domain diagram, boundary nomenclatures and characteristic dimensions of the problem.

\[
\begin{align*}
\hat{\sigma} &= \frac{\sigma}{\sigma_c}, \quad \text{current density by } j_c = k_0 E_c \left( \hat{\mathbf{j}} = \frac{\mathbf{j}}{j_c} \right), \quad \text{total emitted current } I \text{ by } j_c r_0^2, \\
\hat{\mathbf{u}} &= \frac{\mathbf{u}}{u_c}, \quad \text{velocity by } u_c = \frac{\mathbf{u}}{u_c}, \\
\text{and temperature by } T_0.
\end{align*}
\]
### Table 1: Non-dimensionalized bulk equations

<table>
<thead>
<tr>
<th>Equation Name</th>
<th>Equation</th>
<th>Domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maxwell-Poisson</td>
<td>$\nabla \cdot \left( \varepsilon_r \hat{E} \right) = \hat{\rho}_{ch}$</td>
<td>$\Omega_l \cup \Omega_v$</td>
</tr>
<tr>
<td>Maxwell-Faraday</td>
<td>$\nabla \times \hat{E} = 0 \rightarrow \hat{E} = -\nabla \phi$</td>
<td>$\Omega_l \cup \Omega_v$</td>
</tr>
<tr>
<td>Charge conservation</td>
<td>$\nabla \cdot \hat{j} = \nabla \cdot \left( \left( 1 + \Lambda \left( \hat{T} - 1 \right) \right) \hat{E} \right) = 0$</td>
<td>$\Omega_l$</td>
</tr>
<tr>
<td>Mass conservation</td>
<td>$\nabla \cdot \hat{u} = 0$</td>
<td>$\Omega_l$</td>
</tr>
<tr>
<td>Momentum conservation</td>
<td>$\varepsilon_r^2 \hat{W} \left( \hat{u} \cdot \nabla \right) \hat{u} = \nabla \cdot \left( -\hat{p} \mathbb{I} + \varepsilon_r C_a \sqrt{B} \frac{\left( \hat{j} \hat{j} \right)}{1 + \Lambda (\hat{T} - 1)} \left( \hat{\nabla} \hat{u} \cdot \hat{u} + \hat{\nabla} \hat{u}^T \right) \right)$</td>
<td>$\Omega_l$</td>
</tr>
<tr>
<td>Energy conservation</td>
<td>$\varepsilon_r G \frac{\varepsilon_r^2}{\sqrt{B}} \hat{u} \cdot \hat{\nabla} \hat{T} = \frac{\varepsilon_r^2 H}{\varepsilon_r B} + \frac{\left( \hat{j} \hat{j} \right)}{1 + \Lambda (\hat{T} - 1)}$</td>
<td>$\Omega_l$</td>
</tr>
</tbody>
</table>

### Table 2: Non-dimensionalized equations fulfilled on the meniscus interface $\Gamma_M$

<table>
<thead>
<tr>
<th>Equation Name</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge conservation</td>
<td>$j_n^\prime = \left( 1 + \Lambda \left( \hat{T} - 1 \right) \right) \hat{E}_n^\prime + K_C B \frac{\varepsilon_r}{\varepsilon_r - 1} \left( \hat{\sigma} \hat{\nabla} \hat{u} \cdot \hat{n} - \hat{u} \cdot \hat{\nabla} \hat{S} \hat{\sigma} \right)$</td>
</tr>
<tr>
<td>Surface charge jump condition</td>
<td>$\hat{\sigma} = \hat{E}_n^\prime - \varepsilon_r \hat{E}_n^l$</td>
</tr>
<tr>
<td>Equality of tangential components of the electric field</td>
<td>$\hat{E}_n^\prime = \hat{E}_n^l$</td>
</tr>
<tr>
<td>Kinetic law for charge evaporation</td>
<td>$j_n^\prime = \frac{\hat{\sigma}}{\varepsilon_r} \exp \left( \frac{-1}{\varepsilon_r \sqrt{\hat{T}}} \left( 1 - B \frac{\sqrt{\hat{E}_n^l}}{\varepsilon_r} \right) \right)$</td>
</tr>
<tr>
<td>Equilibrium of stresses in the tangential direction</td>
<td>$\frac{\varepsilon_r C_a \sqrt{B}}{1 + \Lambda (\hat{T} - 1)} \hat{\nabla} \hat{u} \cdot \hat{u} + \hat{\nabla} \hat{u}^T \cdot \hat{n} = \frac{\hat{\sigma}}{\varepsilon_r} \hat{E}_l$</td>
</tr>
<tr>
<td>Equilibrium of stresses in the normal direction</td>
<td>$-\hat{p} + \frac{\varepsilon_r C_a \sqrt{B}}{1 + \Lambda (\hat{T} - 1)} \hat{n} \cdot \hat{u} = \hat{E}_n^\prime - \varepsilon_r \hat{E}_n^l + \left( \varepsilon_r - 1 \right) \hat{E}_l^2 - \frac{1}{2} \hat{\nabla} \cdot \hat{n}$</td>
</tr>
<tr>
<td>Mass conservation of ions evaporated</td>
<td>$\hat{u} \cdot \hat{n} = j_n^\prime$</td>
</tr>
<tr>
<td>Thermal insulation</td>
<td>$\hat{n} \cdot \hat{\nabla} \hat{T} = 0$</td>
</tr>
</tbody>
</table>
Non-dimensional numbers

\[ We = \frac{pu^2r^*}{\gamma} \] Weber number. Ratio of characteristic inertial fluid stresses to surface tension stresses in the emission region.

\[ K_e = \frac{\gamma c_r}{\rho u^* r^*} \] Ratio of the charge relaxation time \( \left( \frac{\gamma c_r}{k_0} \right) \) to the characteristic residence time of liquid \( \left( \frac{\rho u^*}{\gamma} \right) \) in the meniscus tip.

\[ \psi = \frac{\Delta G}{k_B T} \] Ratio of solvation energy \( \Delta G \) and characteristic thermal molecular energy \( k_B T \).

\[ Ca = \frac{\rho_0 u^* r^*}{\gamma} \] Capillary number. Ratio of viscous drag stresses to surface tension stresses in the emission region.

\[ B = \frac{r^*}{r_0} \] Fraction of characteristic emission size \( r^* \) to with respect to radius of the fluid channel \( r_0 \).

\[ Gz = \frac{\rho_0 u^* r^*}{k_T} \] Graetz number. The ratio of characteristic convective \( \left( \frac{\rho_0 u^* r_0}{k_T} \right) \) and conductive \( \left( \frac{k_T r_0}{r^*} \right) \) heat transfer magnitudes.

\[ \Lambda = \frac{k_T r_0}{\gamma} \] Non dimensional sensitivity of the electric conductivity to changes in temperature.

\[ \chi = \frac{k_0}{k_B T} \] Ratio of the kinetic emission time \( \left( \frac{k_0}{k_B T} \right) \) to the characteristic charge relaxation time in the liquid \( \left( \frac{\gamma c_r}{k_0} \right) \).

\[ H = \frac{(r^* / r_0)^2}{k_B T} \] Ratio of the order of magnitude of Ohmic heat dissipation \( \left( \frac{r^*}{\kappa} \right) \) and that of the conductive heat transfer.

4. Boundary conditions

- Energy transport: \( \nabla \hat{T} \cdot \hat{n} = 0 \) on \( \Gamma^I_L \) and \( \hat{T} = 1 \) on \( \Gamma^I_D \).

- Electrodynamics: \( \hat{\phi} = 0 \) on \( \Gamma_I \cup \Gamma^I_D \cup \Gamma^I_R \), \( \hat{\phi} = -\hat{E}_0 \hat{n}_0 \) on \( \Gamma_U \) and \( \hat{\nabla} \hat{\phi} \cdot \hat{n} \) on \( \Gamma^I_L \cup \Gamma^I_U \cup \Gamma^I_R \).

- Hydrodynamics: the fluid enters the computational domain as fully developed pipe flow at the inlet \( (\Gamma_I) \), with a pressure \( \hat{p} = \hat{p}_r + \Delta \hat{p} \) and \( \hat{\vec{u}} \cdot \hat{n} = 0 \). Where \( \hat{p}_r \) is the pressure at the reservoir and \( \Delta \hat{p} = \hat{I} C_R \) is the non-dimensional pressure drop caused by the friction of the fluid with the walls. Where \( C_R = \frac{k_0 \hat{E}_0 \hat{r}_0}{2 \gamma p^*} \) is the non-dimensional value of the tip hydraulic impedance \( (Z_{tot}) \). \( C_R \) will be given by the model in section B. The fluid does not slip on the walls, thus \( \hat{\vec{u}} = 0 \) on \( \Gamma^I_D \).

5. Objective of the problem and numerical procedure

The objective of this problem is to find what is the axisymmetric meniscus shape \( \Gamma^M \) of contact line radius \( r_0 \) that is in static equilibrium supporting steady evaporation of ions, for a given set of input parameters, namely \( B, C_R, \hat{E}_0 \) and \( p_r \). In other words, which is the shape whose associated surface energy or surface tension balances the electric pushing stress and the hydrodynamic fluid stresses for a situation of steady evaporation given the latter inputs and boundary conditions. The solver is initiated with an initial guess of the axisymmetric contour \( (\Gamma^0_M) \), which is generally not in equilibrium. The initial guess is perturbed across several iterations \( (k) \) by using numerical minimization techniques. These perturbations will approach this \( \Gamma^k_M \) towards its equilibrium position.

The solver is comprised of four components, the first three parts enforce equations belonging to a particular physics, that is: electric, fluid, and energy transport problems. The electric solver yields the distribution of electric fields along the meniscus \( \left( \hat{E}^V, \hat{E}^I \right) \) and the surface charge \( (\sigma) \). From there, the electric stress tensor can be computed \( (\hat{\tau}_e) \), the distribution of current density that is being evaporated at the surface \( j'_{e,n} \), and the total current evaporated \( \left( I = \int_{\Gamma_M} j'_{e,n} d\Gamma_M \right) \). The fluid solver yields the velocity field \( (\hat{\vec{u}}) \) and pressure distribution \( (p) \) along the surface of the meniscus. From there, the viscous stress tensor is calculated \( (\hat{\tau}_m) \). The energy transport solver yields the temperature distribution along the computational domain \( (T) \). The temperature plays a substantial role in both the fluid and electric problems, as the electrical conductivity \( (k) \) and fluid viscosity \( (\mu) \) are strong functions of the temperature. The last component of the solver uses the previously calculated tensor distributions and current to guess another \( \Gamma^k_M \) that is closer to the equilibrium condition.
B. Differential Hydraulic Impedance Model of Porous Substrates

State of the art ionic electrospray propulsion system (iEPS) emitter arrays fabricated by the Space Propulsion Laboratory at Massachusetts Institute of Technology constitute of 480 emission sites over 1 mm$^2$. The emitter array is a porous substrate, providing passive propellant flow, via capillary action, to the apex of the emitter tips. The emitter tips are packaged in a hexagonal configuration with 450 µm pitch between individual emitters. Subsequently, the unit cell of an emitter tip is defined as the effective hexagonal cut through the bulk of the porous substrate, which solely supplies propellant to the emission site and the residing emitter tip. Within each unit cell, the propellant must be transported through the bulk substrate. However, at the emitter tip, the propellant can be fed both externally and internally through the emitter tip.

From experimental operation of iEPS emitters it has been shown that the combination of flow rate, propellant characteristics (EMI-BF$_4$) and geometry of the thrusters are such that the resulting Reynolds number is $R_e \ll 1$. Thereby, making Darcy’s law the preferred model to determine the hydraulic impedance of iEPS emitters.

Darcy’s law is the hydraulic equivalent of $V = IR$, Eq. 8, where the potential is replaced by a pressure difference, $\nabla P$. The hydraulic equivalent of current is volumetric flow, $Q$, and for the electric resistance, it is the hydraulic impedance, $Z$. Furthermore, the law states that the impedance is a combination of propellant properties, geometrical ones, and material properties. Here $\mu$ is the dynamic viscosity, $t$ is the thickness of the porous sample, $A$ is the cross-sectional area and permeability is represented as $\kappa$.

$$Q = -\frac{\kappa A}{\mu t} \nabla P = -\frac{\nabla P}{Z} \quad (8)$$

With Darcy’s law, the internal impedance through the porous substrate is trivially found, Eq. 9 is the impedance through the base of the porous substrate, while the impedance through the emitter tip is numerically integrated as the cross-sectional area is location dependent.

$$Z_{\text{bulk}} = \frac{\mu t_{\text{bulk}}}{\kappa A_{\text{bulk}}} \quad (9)$$

G. L. R. Mair derived an analytical equation of the hydraulic impedance for externally wetted emitter tips with a rough surface, Eq. 10. Mair assumed the circumference of a needle had groves of size $D_g$ equally distributed along the perimeter. The equation tracks two sources of impedance, along a cylindrical, e.g. shank, section, and a parabolically shaped tip. The length and radius of the cylindrical section are $L_{\text{shank}}$ and $R_{\text{shank}}$ respectively. The emitter tip is characterized by its height $h$, half-angle $\alpha$, and the radius of curvature of the apex of the tip $R_c$.

$$Z_{\text{ext}} = 4\mu \frac{\pi^2 D_g^3}{9} \left( \frac{L_{\text{shank}}}{R_{\text{shank}}} + \frac{\ln(1 + \tan(\alpha)h/R_c)}{\tan(\alpha)} \right) \quad (10)$$

Darcy’s law and Eq. 10 define the respective impedance of a unit cell of an emitter tip, however, the total hydraulic impedance has the circuit equivalent of the bulk impedance is run in series with the impedance of an emitter tip. The wetting of the emitter tip can be viewed as the internal and external impedance are operated in parallel. Hence, the total impedance of a unit cell is defined as Eq. 11:

$$Z_{\text{tot}} = \left( \frac{1}{Z_{\text{ext}}} + \frac{1}{Z_{\text{int}}} \right)^{-1} + Z_{\text{bulk}} \quad (11)$$

The Kozeny-Carman formula for permeability, Eq. 12 is the conventional permeability model used for the analysis of porous mediums.

$$\kappa_{\text{KC}} = \frac{D_{\text{eff}}^2}{180} \frac{\phi_p^3}{(1 - \phi_p)^2} \quad (12)$$

With $\phi_p$ being the open volume fraction, or porosity, of the porous substrate, and $D_{\text{eff}}$ is the effective diameter of the solid particles forming the permeable medium. Glover relation, $D_{\text{eff}} \sim \Theta D_{\text{pore}}$, is used to relate the particle size to the pore size, $D_{\text{pore}}$. Consequently, assuming the particle distribution to be monodisperse, $\Theta$ is a monotonic function of the porosity, via $\Theta = 0.87 \phi_p^{-3/2}$. In conclusion, the relationship between permeability and pore size is Eq. 13.
The iEPS emitter tips are not fabricated to have special external wetting surface features, therefore, the external wetting is driven by the open channels that were occupied by substrate particles prior to fabrication. Using Glovers relation $D_g$ of Eq. 10 is approximated as:

$$D_g = 0.87 \frac{D_{pore}}{\phi_p^{3/2}}$$

(14)

The domain of a unit cell can now be uniformly discretized into slices of finite thickness each with a constant cross-sectional area to estimate the hydraulic impedance of iEPS emitter tips; via Eq. 9 and Eq. 10, where each slice is treated as a thin shank.

IV. Results

Figure 3 shows the computed stability region for two values of the hydraulic impedance coefficient as a function of the non-dimensional electric field $\tilde{E}_0$ and the non-dimensional contact line radius $\tilde{R}$. This implementation of [3] shows three different regions in the stability diagram of figure 3. The first region holds for a combination of electric fields smaller than a threshold value of $\tilde{E}_0 \sim 0.5$. In this situation, the menisci do not emit current and form a parabolic shape as seen in figure 4a. No statically stable solution in the region between the two dashed lines ($\tilde{E}_0 \in [0.5, 0.59]$) was found, where Coffman [3] identified a transition region; presumably pulsating solutions. For values of the electric field greater than $\tilde{E}_0 = 0.59$, a family of emitting solutions was found; see figure 4b that are sharper than the non-emitting ones. It is noted that the modeled emitting shapes differ substantially from Taylor cones. When the hydraulic impedance is not sufficiently large, the range of electric fields within the stable solution regime drops dramatically for large meniscus sizes.

The results presented in this section have been calculated with reference ionic liquid properties and laboratory conditions, namely $T_0 = 300$ K, $k_0 = 1$ S m$^{-1}$, $k' = 0.04$ S m$^{-1}$K$^{-1}$, $\mu = 10^6$ C kg$^{-1}$, $\mu_0 = 0.037$ Pa s, $k_T = 0.2$ W m$^{-1}$K$^{-1}$, $c_p = 1500$ J kg$^{-1}$K$^{-1}$, $\gamma = 0.05$ N m$^{-1}$, $\Delta G = 1$ eV, and $\rho = 10^3$ kg m$^{-3}$. The non-dimensional numbers yield: $\Lambda = 12$, $\psi = 38.6$, $\chi = 1.81 \cdot 10^{-3}$, $W e = 2.26 \cdot 10^{-6}$, $Ca = 0.026$, $Gz = 0.024$, $K_c = 1.32 \cdot 10^{-4}$ and $H = 0.176$.

Figure 3: Stability boundaries as a function of $\tilde{E}_0$ and $\tilde{R}$ for two different values of hydraulic impedance and $\tilde{p}_r$. Due to computational capability constraints, we infer the emitting stability region for a material with a $C_R = 5 \cdot 10^3$ by interpolation of the two boundaries in the dotted line.
Non emitting parabolic-like meniscus shapes. These shapes are characteristic from the left side of the stability diagram in figure 3.

Emitting meniscus shapes. These shapes are characteristic from the right side of the stability diagram in figure 3.

Figure 4: Non dimensional meniscus shapes as a function of several values of the electric field. The values of the operational space used in this figures are $B = 0.0467$, $\bar{\rho}_r = 0$ and $C_R = 10^3$.

### Table 3: Material properties of each substrate, their respective geometrical relations of the emitter tips, impedance estimations and is pure ionic regime operation expected

<table>
<thead>
<tr>
<th></th>
<th>Borosilicate Glass</th>
<th>Carbon Aerogel</th>
<th>Varapor100</th>
<th>Fused Silica</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$ [°]</td>
<td>26.5</td>
<td>13.5</td>
<td>22.5</td>
<td>30</td>
</tr>
<tr>
<td>$D_p$ [nm]</td>
<td>~2000</td>
<td>900</td>
<td>~100</td>
<td>430</td>
</tr>
<tr>
<td>$\phi_p$ [-]</td>
<td>0.463</td>
<td>0.433</td>
<td>0.47</td>
<td>~0.40</td>
</tr>
<tr>
<td>$D_g$ [nm]</td>
<td>6880</td>
<td>2260</td>
<td>~270</td>
<td>1480</td>
</tr>
<tr>
<td>Pitch [µm]</td>
<td>450</td>
<td>450</td>
<td>450</td>
<td>450</td>
</tr>
<tr>
<td>$h$ [µm]</td>
<td>270</td>
<td>250</td>
<td>330</td>
<td>390</td>
</tr>
<tr>
<td>$t_{base}$ [µm]</td>
<td>730</td>
<td>750</td>
<td>670</td>
<td>610</td>
</tr>
<tr>
<td>$R_c$ [µm]</td>
<td>15.5</td>
<td>10</td>
<td>4</td>
<td>19</td>
</tr>
<tr>
<td>$q/m$ [C/g]</td>
<td>$72.5^{15}$</td>
<td>$44^{22}$</td>
<td>$360^{19}$</td>
<td>$43^{19}$</td>
</tr>
<tr>
<td>$Z_{tot}$ [kg/m^4s]</td>
<td>$1.3 \times 10^{16}$</td>
<td>$2.1 \times 10^{17}$</td>
<td>$3.8 \times 10^{17}$</td>
<td>$4.0 \times 10^{19}$</td>
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<tr>
<td>$Z_{ext}$ [kg/m^4s]</td>
<td>$1.9 \times 10^{16}$</td>
<td>$5.9 \times 10^{17}$</td>
<td>$1.5 \times 10^{18}$</td>
<td>$4.6 \times 10^{20}$</td>
</tr>
<tr>
<td>$Z_{int}$ [kg/m^4s]</td>
<td>$3.1 \times 10^{16}$</td>
<td>$3.4 \times 10^{17}$</td>
<td>$4.9 \times 10^{17}$</td>
<td>$4.6 \times 10^{19}$</td>
</tr>
<tr>
<td>Approximate $C_R$</td>
<td>$6.4 \times 10^2$</td>
<td>$3.2 \times 10^2$</td>
<td>$1.7 \times 10^4$</td>
<td>$3.0 \times 10^3$</td>
</tr>
<tr>
<td>PIR</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
</tbody>
</table>

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Material properties of the four porous substrates under considerations are referenced, directly measured or approximated. The emitter tips geometries that are being investigated are illustrated in Fig. 5. Table 3 summarizes the material properties, geometries of each emitter tip and the modeled hydraulic impedances, via the mathematical framework developed in section B. It is assumed the combined thickness of the bulk substrate and the emitter tip height is 1000µm. Furthermore, the firing mode of the emitters are approximated based on their respective impedance values, with borosilicate glass being the only material not expected to operate in the PIR. That conclusion is confirmed via comparison of the substrates respective empirical \( q/m \) values, the carbon aerogel, Varapor100, and fused silica have a charge to mass ratio of \( \sim 400 \text{ C/g} \) in line with PIR operation, whilst borosilicate glass has operated with the resulting ratio of \( 72.5 \text{ C/g} \). The approximate value of \( C_R \) is presented for each material. The \( C_R \) value is dependent on the characteristic meniscus anchoring size which cannot be trivially linked to emitter geometry (see section V). It is assumed to be equal to \( R_c \). For this analysis the propellant of choice is EMI-BF4, due to its common use in the literature, \( \mu \) has a dynamic viscosity, \( \mu \), of 38 mPas.

![Figure 5: SEM images of the emitter tips utilized to simulated their respective hydraulic impedance’s](image)

Analytical sensitivity analysis of the governing hydraulic impedance equations, external wetting Eq. 10 and internal wetting of the emitter tip. Revealing the importance of the selection of a porous substrate. The driving parameters of the total hydraulic impedance are the \( D_p \), \( D_g \) and \( R_c \). Here, the pore size and groove size have been assumed to be monotonically correlated to each other. Therefore, the upper limit on
Figure 6: Comparison how the internal impedance evolves along the propellant flow path, relative heights of each substrates emitter tips can be clearly identified.
the pore size of borosilicate glass to operate in the PIR is $\sim 600$ nm, i.e., one-third of its current size.

Darcy’s law facilitates a relationship between hydraulic impedance and emitter current, that can be inferred. Assuming the applied pressure is constant, and therefore the product of impedance and volumetric flow rate must remain constant. By mapping the volumetric flow rate into the current emission, $I_{em}$, the following relationship is achieved:

$$I_{em} \propto \frac{q/m \rho}{Z_{tot}}$$

(15)

Empirically it has been shown that there are two ranges of values $q/m$ can take. In PIR $\sim 400$ C/g and in the mixed regime $< 100$ C/g, as shown in Table 3 (less than 10 C/g for pure droplet regime). With increasing hydraulic impedance, the emitted current is expected to decrease due to the inverse relationship (assuming constant geometry and external electric field in steady-state operation).

![Figure 7: Scaled current $I_{em}/I_s$ as a function of the non-dimensional electric field increase $E_0/E_{0s}$.](image)

Figure 7 illustrates the experimental current-voltage plots for Varapor100 and fused silica. The current-voltage plot curves have been scaled according to the starting voltage or starting electric field ($V_s$, $E_{0s}$ respectively). The starting voltage can be considered as the voltage where a linear behaviour of the current with increasing the potential bias begins. Due to the linearity of the electrostatics problem far away from the meniscus, it can be considered as $V - V_s = \frac{E_{0s} - E_0}{E_{0s}}$. $I_s$ is the current emitted when $E = E_{0s}$, or $V = V_s$.

Despite the difficulty of getting information about the meniscus size on the experiment, the computational framework is able to replicate the trends observed regarding the dependence of the current emitted with the $C_R$. Higher hydraulic impedance, while originating more stable menisci with electric field variations, generates lower current outputs.

V. Limitations

The leaky-dielectric model has limited capabilities to replicate experimental conditions. Foremost, the geometry of the electrodes is substantially simplified in order to reduce the size of the operational space. In this paper flat electrodes and a pinned meniscus contact line with the electrode rim are exclusively considered. The pinning radius is understood as the computational parameter to characterize the meniscus size. Real electrode shapes are curved and irregular due to the porosity of the material, which exacerbates the difficulty of inferring the actual contact line pinning radius with the electrodes in experimental conditions. Furthermore, the model only assumes static equilibrium, thus the boundaries of stability may be reduced when including dynamic meniscus behavior.
VI. Conclusion

In this paper, a multi-physics computational framework is presented that aims to inform the design of future electrospray thrusters operating in the PIR with ionic liquids. It is well known that ILIS emission characteristics are highly dependent on the emitter geometries and hydraulic impedances. The computational framework presented includes a numerical model capable of calculating the emitters’ total hydraulic impedance from the tip geometry, the substrates microscopic properties and the dynamic viscosity of the propellant. And a multi-physics model capable of predicting properties useful for propulsion, such as current emitted or static stability range, utilizing hydraulic impedance information and physical properties of ionic liquid propellant. The computational framework unveils that a static pure ion emission is only allowed for microscopic meniscus sizes unless the emitter’s hydraulic impedance is sufficiently high. The increase of material hydraulic impedance generally implies a reduced emitted current for a given external applied potential.

Future work will be centered on the experimental validation of the computational framework, identifying a relation of meniscus characteristic sizes to actual geometrical parameters of the tips, the exploration of feasible thruster operation in the distinct regions of the stability diagram and increasing the fidelity of the differential hydraulic impedance model to account for material heterogeneity and arbitrary distribution of pore sizes.

After validation of the framework, the designer could firstly choose a point in the operational space according to the mission requirements, for instance, current emitted or specific impulse. The framework would provide the designer with a range of feasible hydraulic impedances, geometrical constraints (e.g., pore size, tip radius of curvature) and range of operating voltages to ensure the stability of emission while fulfilling the mission requirements. This physics-based approach should shed light on the design trade-offs of emitter tips intended to operate in the PIR with high fidelity information.

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