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Open electric propulsion with an application to thermionic orificed hollow cathodes

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The concept of open data and software for electric propulsion is discussed and exemplified by an open database that contains over 40 years of thermionic orificed hollow cathode experimental data. Because scaling laws for electric propulsion devices must be verified over a wide range of operating conditions, access to data is critical. Examples of statistical analysis that can be performed with the dataset and resulting physical insights are presented. The empirical analysis conducted suggests that the ratio of total to magnetic pressure inside hollow cathodes depends on at most two other non-dimensional parameters and that the value of 3.7 Torr-cm for the total pressure-insert diameter product is likely a sufficient condition for nominal cathode operation. Solutions to increase the sharing of data and software in the electric propulsion community are suggested.

I. Introduction

Electric propulsion (EP) research relies on access to open databases that cover scattering cross sections,[1] atomic spectra,[2] and outgassing data for vacuum systems.[3] Unfortunately, data and software strictly relevant to EP devices are, in general, neither centralized nor readily accessible. In this work, we explore the concept of "open science" for EP. We consider that open science is synonym for transparency of the entire research process. In practice, this can mean *(i)* public release (under appropriate licenses) of publications, data, and software developed by researchers, *(ii)* open peer-review systems, *(iii)* open research processes, and also *(iv)* open standards for data and metadata. This list is not exhaustive, as there exists a variety of definitions of "open science".[4] We will focus here on the core concept of sharing the results of research through the release of data and software.

The derivation of "constant" underlying physical principles (scaling laws) that allows for the design of EP devices for any regime is desirable. Either dimensional reduction analysis or statistical analysis can be used as a first step in uncovering scaling laws. A multi-dimensional symbolic regression analysis can also be used to model some physical aspect of a particular device (*e.g.*, study of the anomalous transport in Hall-effect thrusters[5]). Those analyses, however, require datasets of substantial size and with enough variation to avoid bias toward a particular design. These datasets may be generated by *(i)* a self-consistent numerical model that has been tested and verified across a large variety of experimental cases, or by *(ii)* experimental campaigns that cover a wide variety of operating conditions. In all cases, extensive physical testing is required. This is problematic, especially for large and high-power systems, because tests are expensive and time-consuming for a single institution. It may also not be possible to cover all operating conditions within the framework of a single experiment.

In the case of thermionic, orificed hollow cathodes, we were able to aggregate 40 years of data from the literature. The data covers multiple propellant species, cathode geometries, and operating conditions, and amounts to roughly 460 data points. In many cases, however, access to data may be restricted by publication policies or pricing. For example, access to conference proceedings and manuscripts may be limited for a given institution. While pre-prints help to effectively disseminate data and results, pre-print

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platforms such as arXiv do not represent mechanical and aerospace engineering. Even if data are accessible in a publication, the digitization of figures, data aggregation, and cross-referencing from a large number of sources is time-consuming and decreases the time available for analysis.

In this work, we first describe a database originally built for the study of the insert plasma of orificed hollow cathodes. We then present multiple analyses we conducted that were enabled by the aggregation of this data. We then discuss the necessity of open data and open source in the context of EP, address possible concerns, and propose modest solutions to foster open access.

II. Database

DATA SOURCES We gathered data from the literature and our own hollow cathode operating at up to 307 A of discharge current on argon. The database we assembled contains experimentally measured electron temperature and plasma density profiles, along with total pressure measurements. We also calculated several derived quantities, including the line-averaged electron temperature and "attachment length," or length over which the cathode plasma is able to support thermally limited thermionic emission. The original experimental measurements were digitized, cross-referenced, and aggregated from the following sources: Siegfried and Wilbur's mercury and noble gas cathodes,[6–9] Salhi's cathode[10] operating on both argon and xenon, Friedly's cathode,[11] the T6 cathode,[12,13] Domonkos's cathodes (AR3, EK6, SC012),[14] the NSTAR discharge cathode,[15–17] the NEXIS cathode,[18–20] the JPL 1.5 cm LaB_6 cathode,[21,22] and our own cathode, the Princeton Large Hollow Cathode (PLHC).[23] The method by which we compute the average electron temperature and the "attachment length" is presented in Ref. 24.

STRUCTURE The original proposed Entity Relationship Diagram of the database is shown in Fig. 1. In practice, the database is flattened (all separate tables are joined together) to allow efficient data analysis.

FILE FORMAT In the absence of a server hosting the database, the data are stored in the "Hierarchical Data Format version 5" (HDF5).[25] HDF5 is an open source, cross platform file format that is used across a variety of scientific and engineering disciplines and that features excellent I/O performance.

IMPLEMENTATION The database is built with the Python language and the `Pandas` library.[26] The initial `Pandas` dataframe is constructed from "raw" column-separated value (CSV) files that were generated from literature data. The data are then aggregated into a monolithic, flat `Pandas` frame and saved as an HDF5 file.

III. Applications

A. Evidence of scaling relationship

We have performed an empirical analysis of the cathode total pressure, the details of which are presented in Ref. 27. We share here further insight we obtained thanks to additional pressure data that we gathered on our hollow cathode running at up to 307 A of discharge current.

Statistical tools enable the analysis of large datasets. "Manifold learning" is a non-linear method that is similar to "Principal Component Analysis," which seeks to find the eigenbasis of a high-dimensional dataset via linear decompositions. Manifold learning attempts to uncover the true dimensionality of a dataset by applying a non-linear method that (qualitatively) "unfolds" the dataset. This is equivalent to projecting the dataset onto a smaller dimensional subspace while keeping neighboring data points close to one another.

We show in Fig. 2 the results of the application of the Local Linear Embedding (LLE) manifold learning method[28] implemented in the Python library `scikit-learn`[29] to find a simple projection of our original 7-D non-dimensional pressure dataset onto a 2-D plane. The LLE is calculated with $k = 14$ neighbors with a reported reconstruction error of 7.3×10^{-7}. Although the embedding cannot be used to retrieve the original relationship between the normalized quantities, the collapse of the dataset onto a 2-D curve indicates that the dataset has an underlying two-dimensional structure.

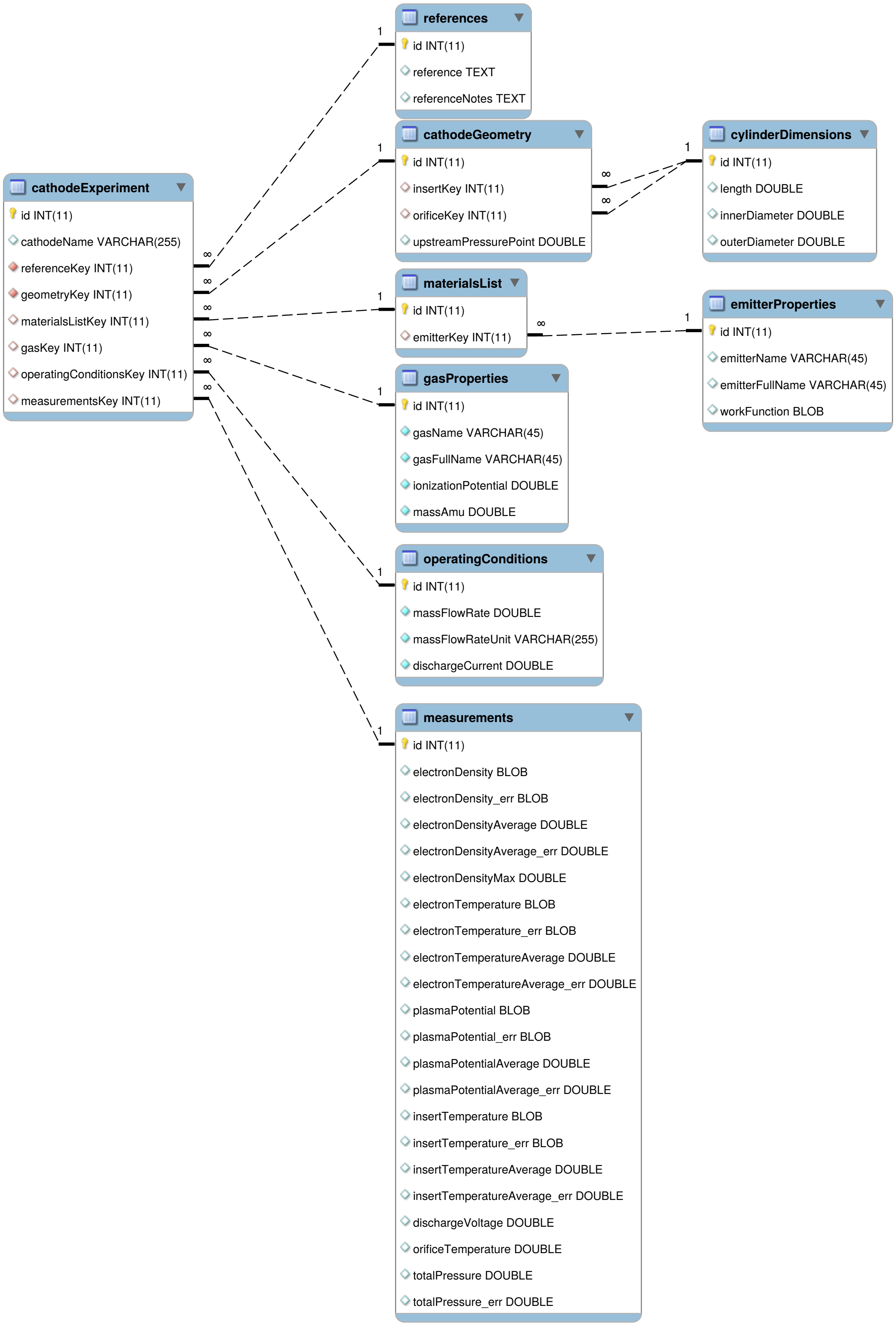

Figure 1: Structure of the database.

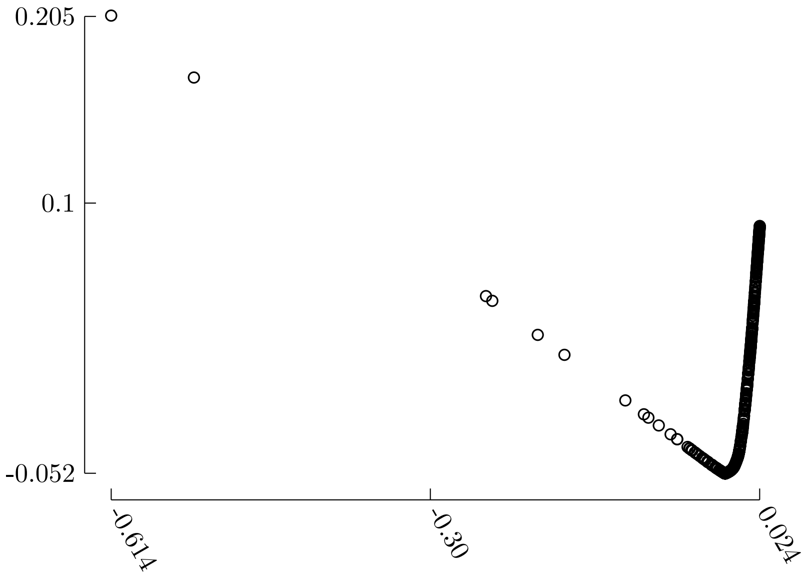

Figure 2: Local Linear Embedding of the normalized 7-D pressure dataset.

Can this 2-D relationship be retrieved from first principles? Under the assumption that the momentum flux of heavy particles on the orifice plate is negligible, the scaling law for the total pressure in cathodes we derived in Ref. 30 from the plasma momentum balance can be re-written as:[23]

$$\frac{P}{P_{mag}} = \frac{1}{4} - \ln \frac{d_o}{d_c} + C \frac{P_{gd}}{P_{mag}}, \tag{1}$$

where $C \approx 3.43$, P is the total pressure, d_o is the orifice diameter, and d_c is the cathode insert diameter. The gasdynamic and magnetic pressures, P_{gd} and P_{mag}, are defined as:

$$P_{gd} = \frac{4\dot{m}a}{\pi d_o^2}, \text{ and} \tag{2}$$

$$P_{mag} = \frac{\mu_0 I_d^2}{\pi^2 d_o^2}, \tag{3}$$

respectively. $\dot{m}$, I_d, μ_0, and a are the mass flow rate, discharge current, vacuum permeability, and gas speed of sound, respectively. Equation 1 indicates that the total pressure in hollow cathodes is a balance between the gasdynamic and magnetic pressures. The relationship as applied to the entire normalized pressure dataset is shown in Fig. 3. Most of the variation is captured by the above relationship. Deviations from the theoretical approximation may be explained by the plasma effects that are neglected in Eqn. 1.

B. Cathode operating envelope

We have shown in Ref. 24 that the pressure-diameter product for a given cathode is close to 4.2 Torr-cm. We show in Fig. 4 updated results that incorporate additional data. With the updated data, the most probable pressure-diameter product is 3.7 Torr-cm.

From the pressure-diameter product and geometry of a cathode it is possible to obtain an estimate of a likely "nominal" mass flow rate, $\dot{m}$. We assume that the total pressure is given by only the neutral species with a neutral gas temperature, T_n, in the range of 2000–4000 K. The total pressure, P, is computed from the stagnation pressure for both the molecular and viscous flow regimes:

$$P = \frac{\dot{m}}{\pi \left(d_o/2\right)^2} \sqrt{\gamma R_g T_n} F\left(\gamma\right), \tag{4}$$

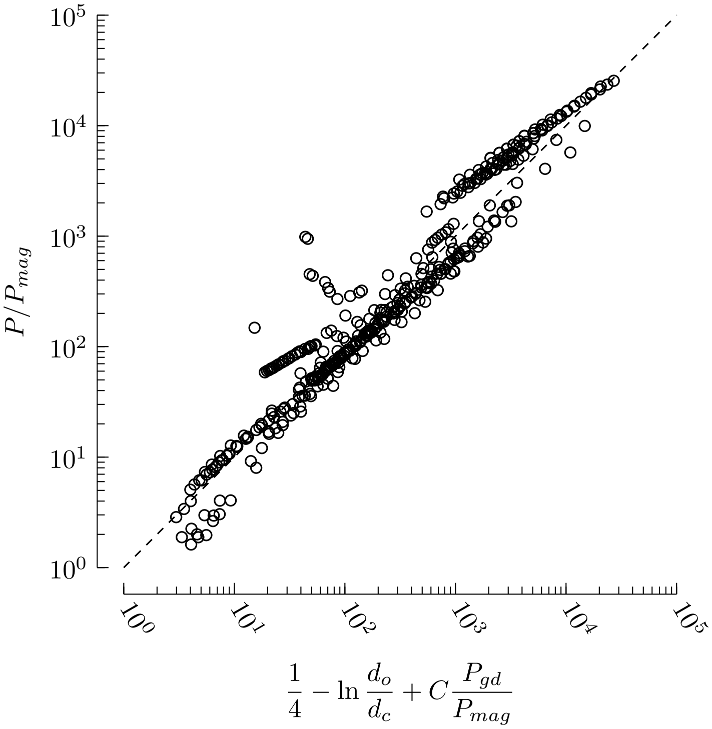

Figure 3: Theoretically derived expression applied to the entire experimental dataset.

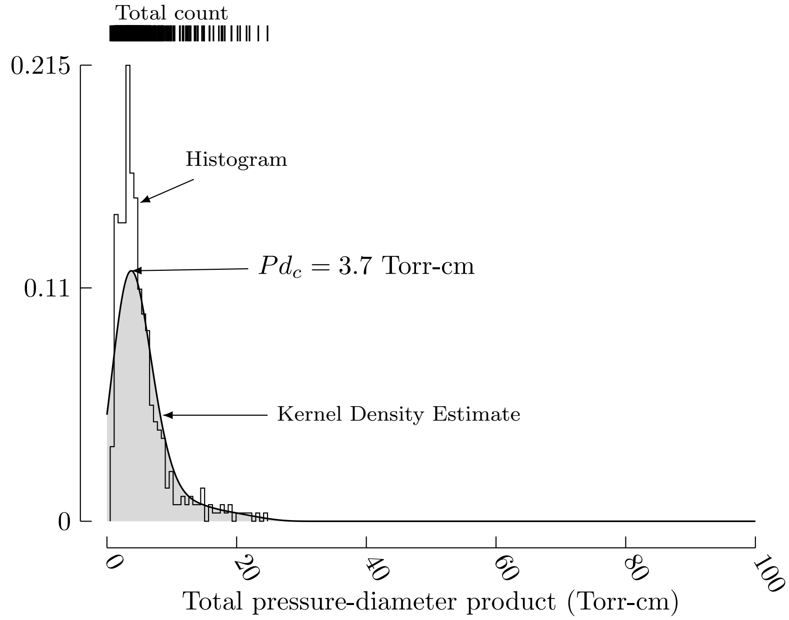

Figure 4: Distribution of total pressure-diameter product for a large number of cathodes. Pressure-diameter product calculated using the orifice diameter for only those cathodes presented in Ref. 14.

where R_g is the specific gas constant. $F(\gamma)$ is a function of the specific heat ratio, γ, only:

$$F_{\text{viscous}} = \frac{1}{\gamma}\left(\frac{\gamma+1}{2}\right)^{\gamma/(\gamma-1)}, \text{ and} \tag{5}$$

$$F_{\text{molecular}} = \frac{\sqrt{2\pi}}{\sqrt{\gamma}}\frac{\gamma+1}{2}. \tag{6}$$

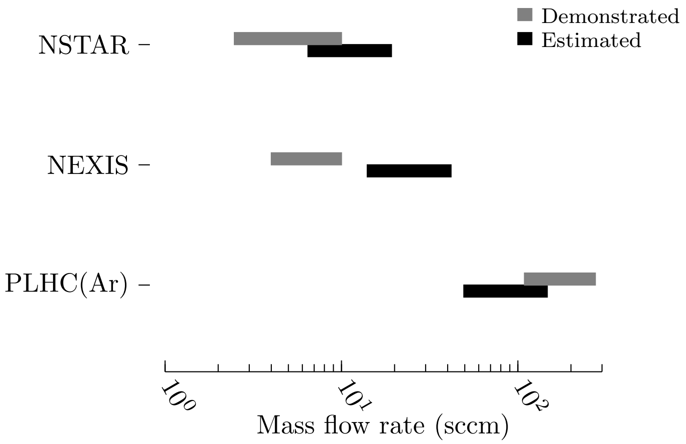

Figure 5: Estimated and demonstrated range of mass flow rate for select cathodes.

We show in Fig. 5 this approach applied to the PLHC and to the NSTAR and NEXIS discharge cathodes, along with the demonstrated range of mass flow rates. The estimated range of mass flow rates overlaps with the demonstrated range for both the NSTAR and our cathode. The agreement is worse for both the NEXIS and our cathode because they operate further from the most-probable pressure-diameter. Our approach also neglects the discharge current contribution to the total pressure, which becomes significant at higher currents. Finally, our cathode typically operates at a much lower temperature than other lanthanum hexaboride cathodes: during operation the cathode tip temperature can be as low as 800°C. The lower operating temperature of our cathode can likely be explained by its large emission area.

IV. Discussion

Open science relies at its core on the public distribution of research data and software. Both should be freely available (we mean here both *libre* **and** *gratis*, or "free as in freedom" **and** "free of charge"[31]) to other researchers. We discuss in this section the benefits of sharing data and software, address possible concerns, and suggest some additional incentives.

A. Open data

The applications shown in the preceding section underline the necessity to openly share data. As mentioned in the Introduction, while EP generally benefits from open data, datasets generated as part of EP research are not often shared with other researchers. This is a major problem, as the lack of access to data and metadata generated by other institutions is an impediment to research.[32,33] We spent a considerable amount of time sifting through a variety of documents to be able to generate the cathode dataset described in Section II. We were sometimes prevented from gathering useful data because of the quality of the scanned documents that are available online. In those instances, the data are lost forever. Having direct access to digitized data (even through multiple sources), not only considerably decreases the time-to-analysis and the possibility of a mistake in data gathering, but also ensures the preservation and consistency of the data.

BARRIERS TO DATA SHARING Recent surveys[32,34–36] indicate that, although researchers view open access to data favorably, there remain barriers to data sharing: *(i)* concern that others may publish an article before the organization that collected data, *(ii)* lack of time and funding to properly document and make data available, *(iii)* lack of data and metadata standards, *(iv)* possibility that the data are misinterpreted, *(v)* uncertainty about copyright, and *(vi)* uncertainty about repository location. However, most researchers are willing to share data if there is formal recognition, at least in the form of citations.[35]

At the individual level, concerns about others publishing journal articles before the primary authors of a given dataset and the data being cited can be addressed by using online data repositories that generate a Digital Object Identifier (DOI) and that provide a time period during which the data cannot be accessed (*i.e.*, an "embargo" period). As in the case of journal publications, the DOI can be used to cite a dataset created by another researcher. As an additional incentive, publications for which data (and also software) are provided are cited more often than those for which no data are available.[37] A list of available data repositories as recommended by the journal *Nature* can be found in Ref. 38.

To ensure that the data are reused, researchers should provide relevant metadata and select an appropriate license.[39,40] Online tools are available to choose the appropriate software and/or data license.[41] The MIT or Apache 2.0 licenses are permissive and allow for commercial reuse, while the GNU Public Licenses (GPL) feature a strong "copyleft" clause which ensures that any derivative work is released under that same license. Commercial and closed-source licenses should be avoided.

The EP community should collectively address the lack of standards for data and metadata, ideally through organizations such as the Electric Rocket Propulsion Society and the AIAA Electric Propulsion Technical Committee. We note that NASA encourages such efforts: "Community-based standards should be promoted. NASA policy should encourage all supported investigators to make use of existing data and metadata standards (format and content standards) whenever feasible."[42]

FURTHER INCENTIVES Beyond the actions of individual researchers, other actors such as the funding agencies, publishers, and the EP community can provide additional incentives to share data. In the United States, federal grants require a data management plan (DMP) and data sharing. NASA encourages the release of data that appear in figures or tables included in publications (either peer-reviewed articles or conference proceedings).[42] Even if the data fall under export control, non-dimensionalization is suggested to allow for the release of some data.[43]

Table 1 shows publisher requirements for journals that cover part of the hollow cathode and EP literature. While encouraging data sharing is a step in the right direction, stronger incentives are needed to ensure that data are shared. Stronger requirements for data must be implemented at the publisher level.

Table 1: Publisher policies for data sharing.

Publisher	APS, IEEE	AIAA, AIP, Elsevier, IOP
Requirement	None	Encouraged

Meaningful actions can be undertaken by the EP community to foster data release. These include, for example, creating standards for data and metadata, requesting stronger publisher requirements, or maybe creating a "best dataset" award for conferences.

B. Open software

Self-consistent numerical models are a critical tool to uncover scaling laws. As in the case of datasets, however, the EP community does not typically share tools developed by researchers. While broad algorithmic descriptions are found in publications associated with a given program, those may not be enough to provide an unambiguous description of the inner workings of the software due to the limitations of natural and algorithmic language semantics.[44] As an example, in the context of EP, we performed a review of hollow cathode models in Ref. 45 but were only able to reproduce a handful of the reviewed models because the descriptions given in the respective publications were inaccurate or not sufficient.

Much like access to data, access to software source code has many benefits.[40] From a scientific stand-point, it ensures that software is beholden to the same standards of peer review as other scientific publications, that results can be reproduced, and that scientific efforts (for strict non-replication studies) are not spent on duplicating already-existing functionality. Researchers are able to peer into and understand the core algorithms of a given program to a degree not granted by simple linguistic explanations[44] and need not trust that the software "black box" performs as described.[46,47] The functionality of the software can also be extended by other researchers. From an engineering stand-point, widely available predictive tools that have been verified with experimental data and independently peer-reviewed are invaluable to institutions and commercial partners for innovative designs.

"Open source" does not exclude commercial participation. A wide variety of open source projects are backed by commercial actors (*e.g.*, Android OS,[48] Red Hat Enterprise Linux OS,[49] OpenFOAM,[50] pfSense[51]). Commercial actors (where not prohibited by regulations, export control, or contractual obligations) can be integrated into open EP software initiatives and can benefit from both access to software and datasets.

C. What can an EP researcher do?

A variety of online tools are available in order to share data, software, and publications. Reference 33 features an extensive list of tools available for researchers. We summarize here some of the suggested tools and propose additional resources.

Data management plans and repositories Researchers should create and follow *data management plans* (DMP) to make sure data are preserved. For academic institutions, libraries are a useful resource to create DMP. Alternatively, online tools can be used to do so (*e.g.*, `https://dmptool.org`). The data should *always* be accompanied by relevant metadata that explains the context and content of the shared data.

Most data repositories generate a DOI that can be added to journal publications. Reference 38 presents a list of repositories along with their respective limits on allowed data size.

Code repositories Version control systems (*e.g.*, SVN, Git, Mercurial) ensure that any edits to text files are tracked. Github (`https://github.com`) and Bitbucket (`https://bitbucket.org`) provide online storage for code or text repositories, along with other features, such as bug tracking, comments, or creation of code releases. Individual academic institutions may also have internal repositories. Some data-oriented repositories (*e.g.*, Zenodo, `https://zenodo.org`) can also be linked directly to a Github repository so that a DOI is generated for software as well. The DOI may then be used to cite a program hosted on Github.

Limit usage of proprietary software To ensure work is reproducible, open source software should be preferred over proprietary systems. The Julia and Python languages along with the Spyder Integrated Development Interface and other Python libraries, for instance, provide excellent alternatives to proprietary systems. These languages and associated libraries are also free and well-supported.

Documentation Best software practices call for code documentation. Beyond thorough code comments, tools to automatically document software include Sphinx (`https://www.sphinx-doc.org`) or Doxygen (`https://www.doxygen.nl`). A "markdown language" should also be used to document datasets.

Publications As mentioned in the Introduction, pre-print repositories dedicated to aerospace engineering are not common. However, online sharing of "post-print" articles is, in most cases, allowed. The "Sherpa Romeo" tool[52] outlines journal policies relevant to the sharing of pre- and post-prints of a publication.

V. Conclusion

We briefly discussed the benefits of open data and open software in the context of Electric Propulsion and provided solutions at multiple levels to incentivize sharing. To illustrate the benefits of open data and science, we have presented a new database for thermionic, orificed hollow cathodes and conducted statistical analyses that were enabled by the aggregation of this data.

We hope that, through sharing both our dataset and associated software and through suggesting tools for others to do the same, EP researchers will follow suit. The EP community has the opportunity to learn from other fields (*e.g.*, genomics) to create standards for metadata, data release, and software release, and benefit from increased access.

Data Availability

The cathode dataset and examples of statistical analysis are available at the following address: `https://doi.org/10.5281/zenodo.3957871`.

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