Electrospray Plume Modeling for Rapid Life and Performance Analysis

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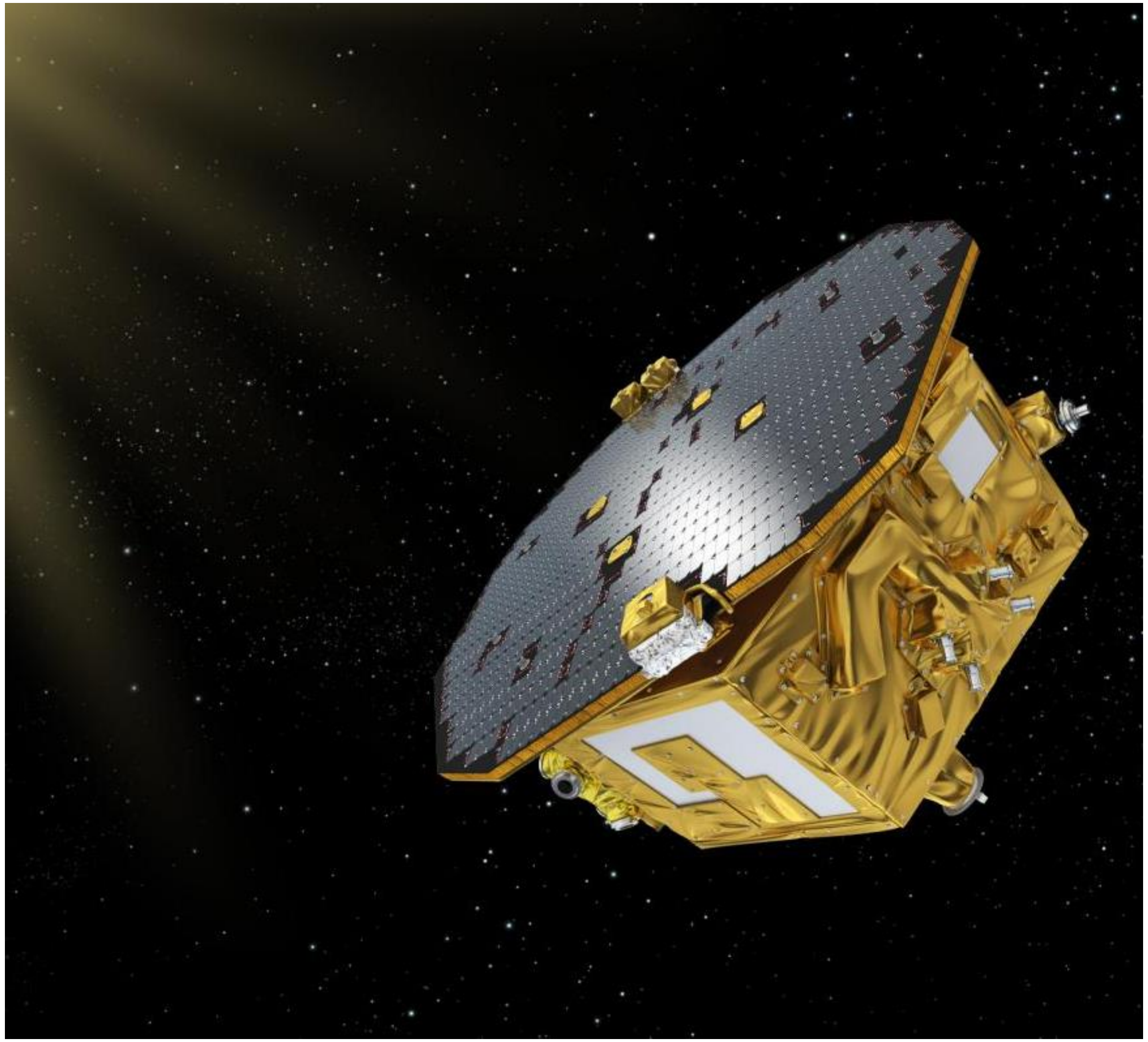
Prof. Richard Wirz
UCLA Plasma and Space Propulsion Laboratory
University of California, Los Angeles

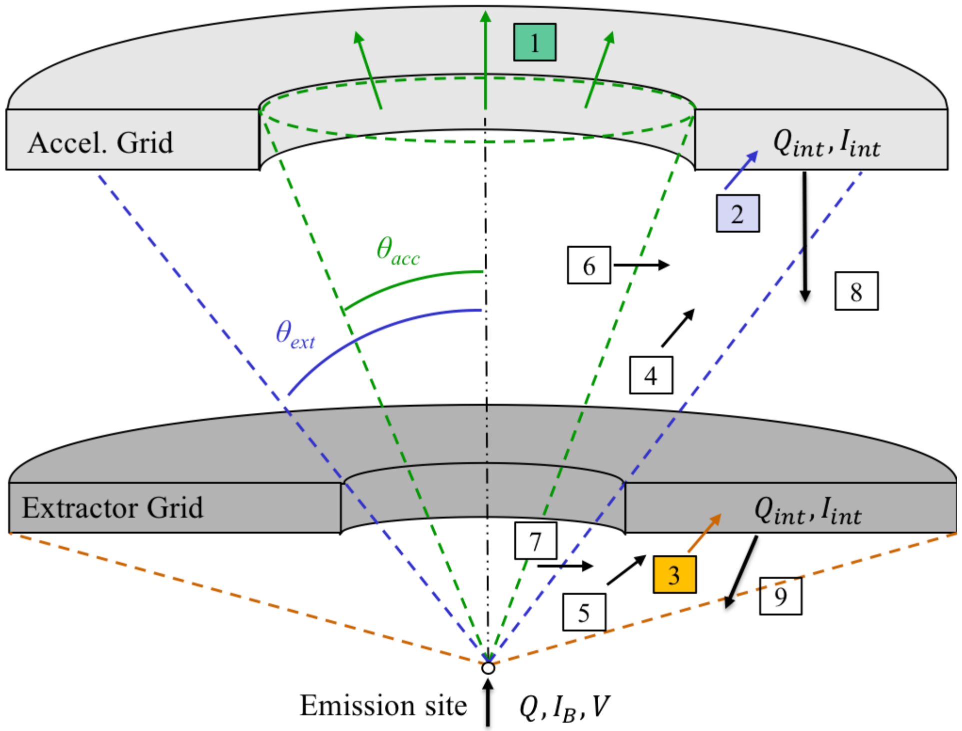
Outline

- Background and Motivation
  - Primary Life-Limiting Failure Mechanisms
  - Experimental Plume Profiles Measurements
- Data-Driven Modeling Approach
  - Physics-based Simulations
  - Surrogate Model
  - Bayesian Inference
- Key Results
  - Sensitivity Analysis
  - Inferred Initial Conditions



LISA Space Mission

Research Motivation



1	T, Thrust from electrospray emission through accelerator grid
2	$\dot{m}_{acc}$, Propellant mass flux toward accelerator grid
3	$\dot{m}_{ext}$, Propellant mass flux toward extractor grid

- Overspray is a primary life-limiting failure mechanism for electrospray thrusters
- <u>Minimizing mass flux</u> towards the extractor and accelerator grids can increase lifetime and thrust
- **Complete characterization of an electrospray plume** by modeling and experiment is necessary to better understand thruster lifetime and performance under various operating conditions

[1] A. Thuppul, P. L. Wright, A. L. Collins, J. K. Ziemer, and R. E. Wirz, "Lifetime Considerations for Electrospray Thrusters," Aerospace, vol. 7, no. 8. 2020
[2] Ziemer, J. K., "Performance of Electrospray Thrusters," 31st International Electric Propulsion Conference, Ann Arbor, MI, USA, 2009, p. pp. 1–13.

Super-Gaussian Mass Flux and Current Density Profiles

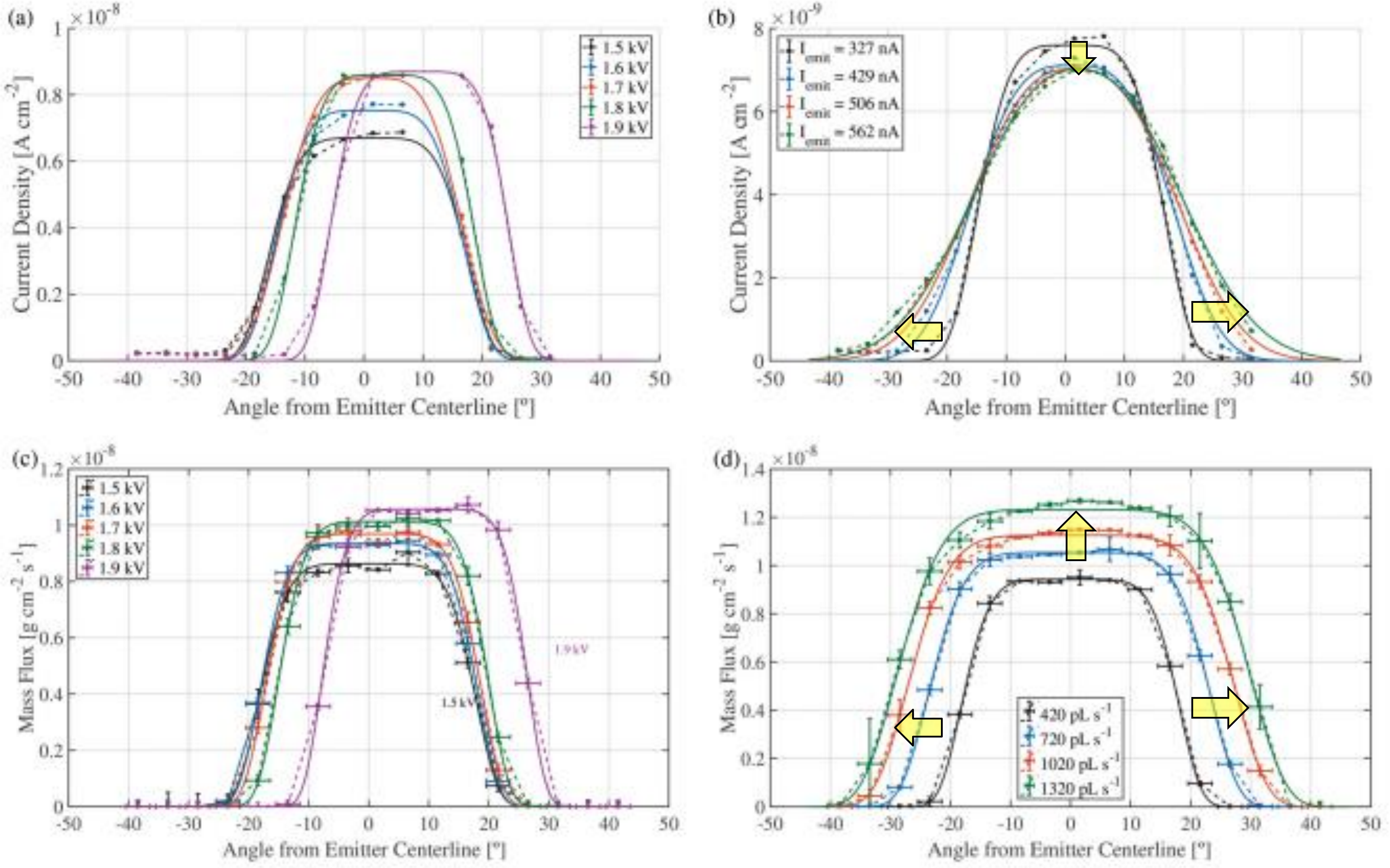


FIG. 3. Current density as a function of half angle for varying (a) extraction voltages (fixed flow rate of 420 pLs^{-1}) and (b) flow rates (constant voltage of 1.6 kV). Mass flux as a function of half angle for varying (c) extraction voltages (fixed flow rate of 420 pLs^{-1}) and (d) flow rates (constant voltage of 1.6 kV). All profiles shown with super-Gaussian fits. The trends of these fits with voltage and flow rates are shown in Fig. 5.

Super-Gaussian Form:

$$p(\theta) = A * \exp\left(-\left(\frac{(\theta-\theta_t)^2}{2\sigma^2}\right)^n\right)$$

A - amplitude

σ – standard deviation

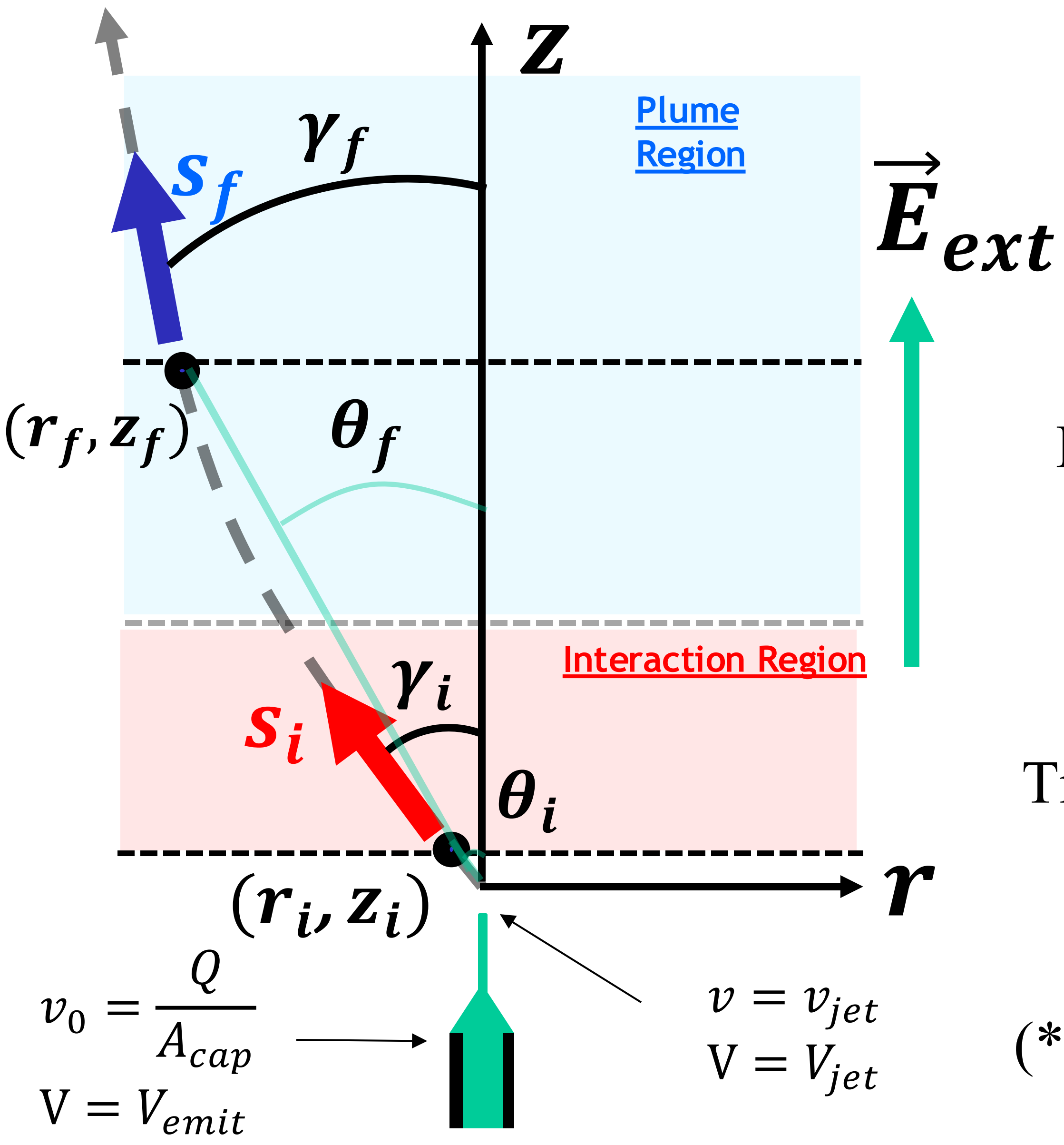
θ – plume angle

θ_t – plume tilt off central axis

n – sharpness (Gaussian for n=1)

Anirudh Thuppul, Peter L. Wright, Adam L. Collins, N. M. Uchizono, and Richard E. Wirz, "Mass Flux and Current Density Distributions of Electrospray Plumes," *Journal of Applied Physics* (2020)

PEPPER – Problem Geometry



$$\boxed{\mathbb{M}_P: \boldsymbol{\theta_i}, \boldsymbol{\gamma_i}, \boldsymbol{V} \rightarrow \theta_f}$$

Charged Particle EOM: $\frac{d^2\vec{r}}{dt^2} = -\frac{q}{m}\nabla\phi$

$\vec{r}(t) = \vec{r}_i + \vec{v}_i t + \frac{1}{2}\frac{q}{m}\vec{E}t^2$

Initial Conditions Needed:

- $\frac{q}{m}$: specific charge
- r_i, z_i: initial positions
- $\vec{v}_i$: initial velocity, where $s_i = |\vec{v}_i|, \gamma_i = \tan\left(\frac{v_r}{v_z}\right)$

Trajectories are the same if: $\frac{KE}{q} = \frac{1}{2}\frac{m}{q}\vec{v}_i^2 = V_{jet} - V_{emit}$

Initial Conditions
(*which *don't* require $\frac{q}{m}$):

θ_i: initial position based on r_i, z_i
γ_i: initial emission angle
V: electrode voltage

Results – COMSOL Charged Particle Tracing

Electric Field Solver:

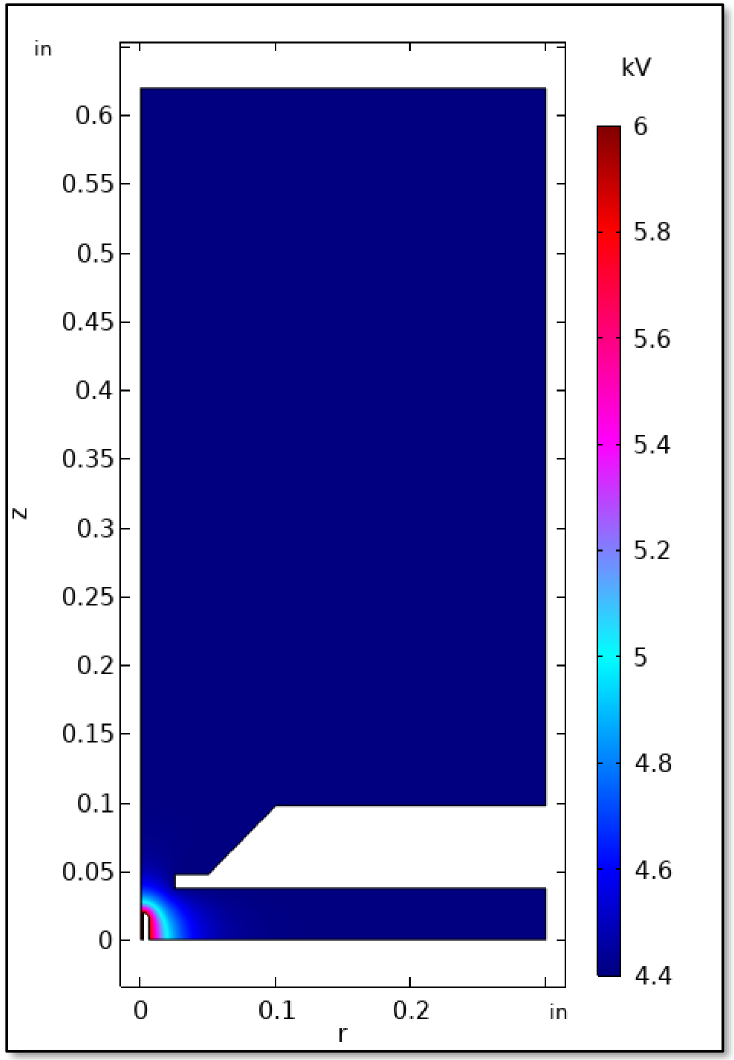
$$\boldsymbol{E} = -\nabla V$$

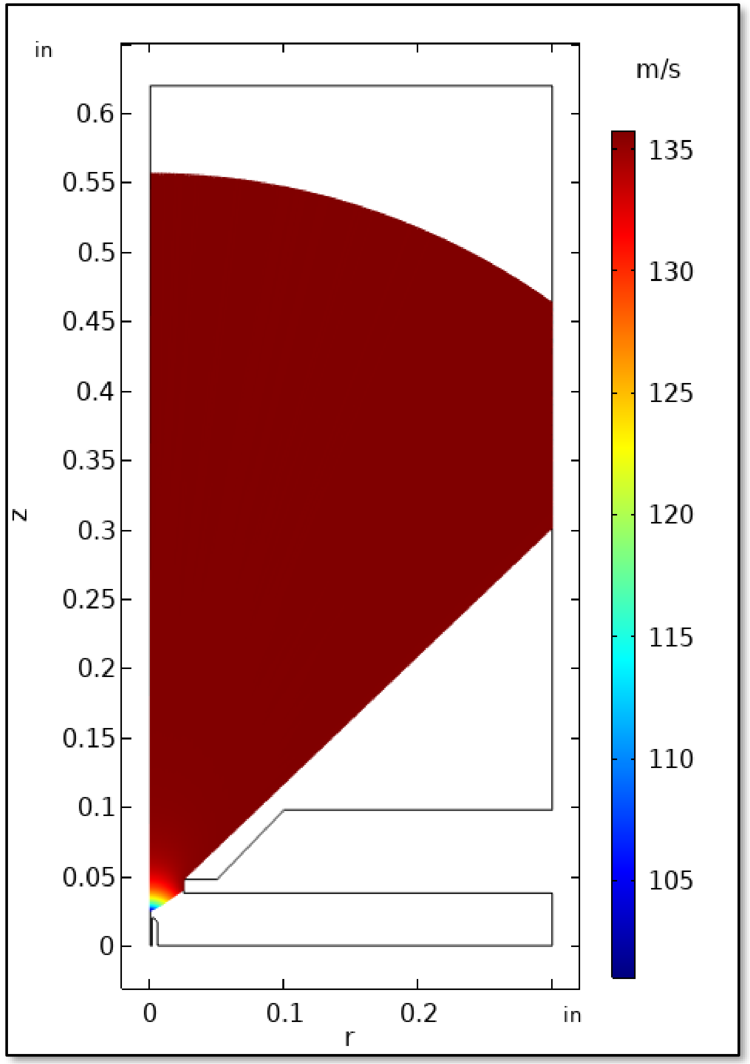
BCs: $V_{emit}, V_{extr}, V_{acc}, V_{beam\ dump}$

Charged Particle Tracing:

$$\frac{d(m_p \boldsymbol{v})}{dt} = \boldsymbol{F}_e = eZ\boldsymbol{E}$$

where e is elementary charge, m_p is the particle mass, and Z is the charge number.





[1] M. Gamero-Castaño, "Characterization of the electrosprays of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide in vacuum," Phys. Fluids, vol. 20, no. 3, p. 32103, Mar. 2008, doi: 10.1063/1.2899658.
[2] M. Gamero-Castaño and A. Cisquella-Serra, "Electrosprays of highly conducting liquids: A study of droplet and ion emission based on retarding potential and time-of-flight spectrometry," Phys. Rev. Fluids, vol. 6, no. 1, p. 13701, Jan. 2021, doi: 10.1103/PhysRevFluids.6.013701.

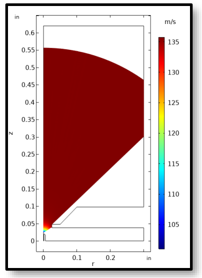
Surrogate Modeling – Polynomial Chaos Expansion

$$Y_{PCE} = \mathbb{M}(\mathbf{X})$$

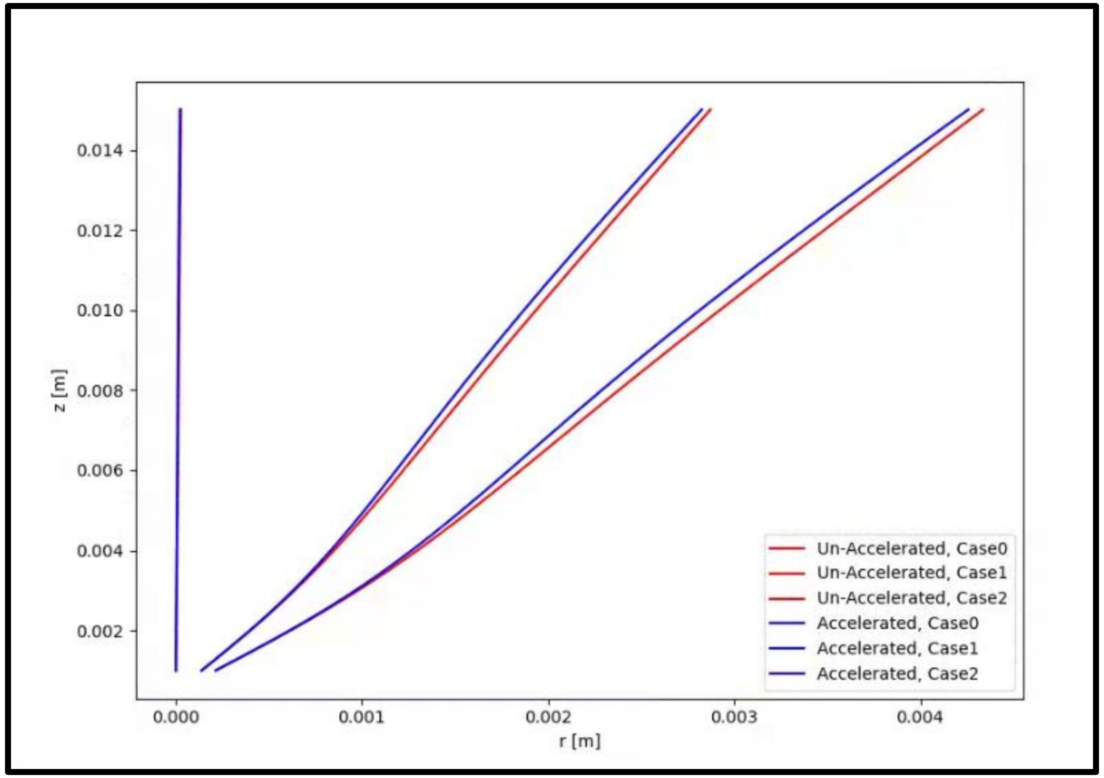
where an analytical "metamodel" model for Y_{PCE} is obtained by sampling some input distribution in $\boldsymbol{X}$ to then map these random (or uncertain) variable inputs to a given quantity of interest.

$$\mathbb{M}(\mathbf{X}) = \sum_{\alpha \in N^d} y_\alpha \Psi_\alpha(\boldsymbol{X})$$

is the functional form of the PCE, where y_α are the coefficients or "mode strengths" and Ψ_α are the basis functions, or "mode functions".



$$\mathbb{M}_P: \boldsymbol{\theta}_\mathbf{i}, \boldsymbol{\gamma}_\mathbf{i}, \mathbf{V}_\mathbf{acc} \rightarrow \theta_f$$

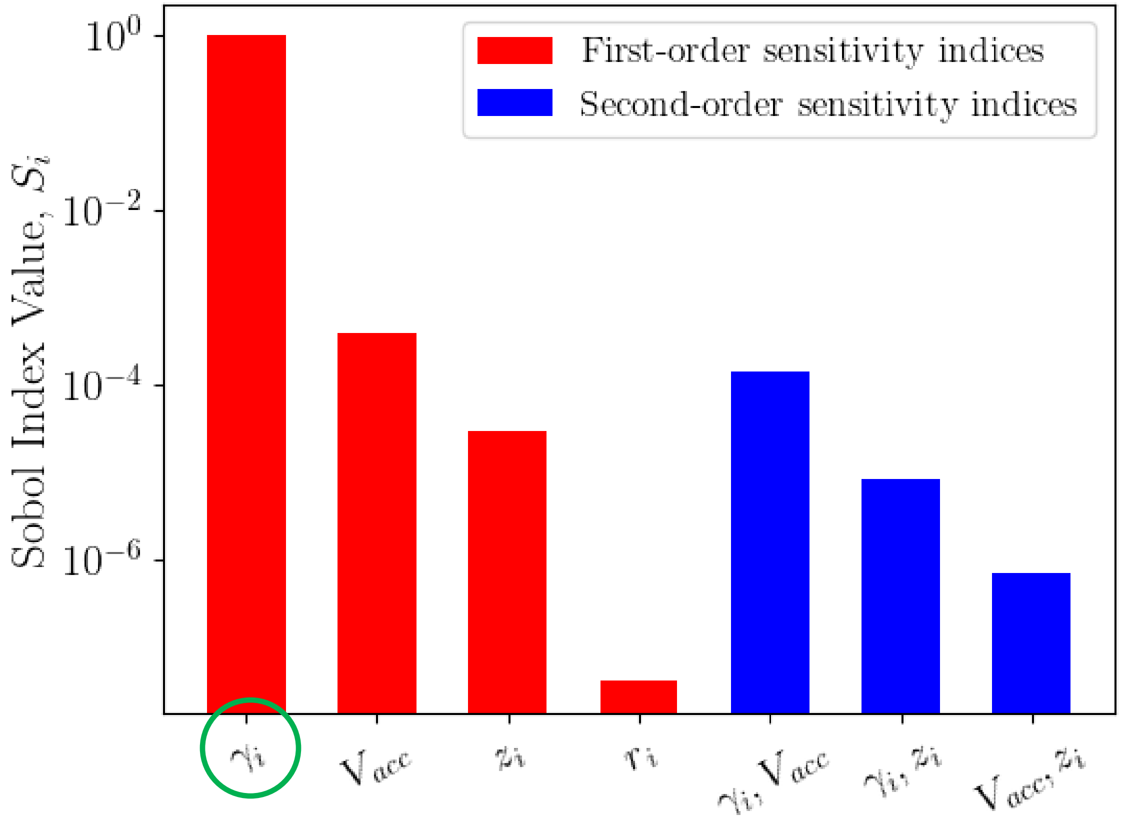


These trajectories are all created from <u>*one* analytical function</u>, namely a Polynomial Chaos Expansion (PCE)

[1] R. Jin, W. Chen, and T. W. Simpson, "Comparative studies of metamodelling techniques under multiple modelling criteria," Struct. Multidiscip. Optim., vol. 23, no. 1, pp. 1–13, 2001, doi: 10.1007/s00158-001-0160-4.
[2] K. Cheng, Z. Lu, C. Ling, and S. Zhou, "Surrogate-assisted global sensitivity analysis: an overview," Struct. Multidiscip. Optim., vol. 61, no. 3, pp. 1187–1213, 2020, doi: 10.1007/s00158-019-02413-5.
[3] D. Shen, H. Wu, B. Xia, and D. Gan, "Polynomial Chaos Expansion for Parametric Problems in Engineering Systems: A Review," IEEE Syst. J., vol. 14, no. 3, pp. 4500–4514, 2020, doi: 10.1109/JSYST.2019.2957664.
[4] E. Torre, S. Marelli, P. Embrechts, and B. Sudret, "Data-driven polynomial chaos expansion for machine learning regression," J. Comput. Phys., vol. 388, pp. 601–623, 2019, doi: https://doi.org/10.1016/j.jcp.2019.03.039.
[5] M. Hadigol and A. Doostan, "Least squares polynomial chaos expansion: A review of sampling strategies," Comput. Methods Appl. Mech. Eng., vol. 332, pp. 382–407, 2018, doi: https://doi.org/10.1016/j.cma.2017.12.019.

Results – Surrogate Modeling

<u>Goal</u>: By how much (relatively) does each input parameter, $\boldsymbol{\theta_i}, \boldsymbol{\gamma_i}$, and $\mathbf{V_{acc}}$, influence the output parameter, $\boldsymbol{\theta_f}$, in $\mathbb{M}_{\mathrm{PCE}}$: $\boldsymbol{\theta_i}, \boldsymbol{\gamma_i}, \mathbf{V_{acc}} \rightarrow \theta_f$?



- Grid impingement is most sensitive to the distribution of **initial emission angles** of droplets entering the plume region domain

Quantitative results showing a <u>sensitivity analysis</u> of model input parameters using <u>variance-based Sobol indices</u>

Results – Bayesian Inference ← Super-Gaussian Profiles

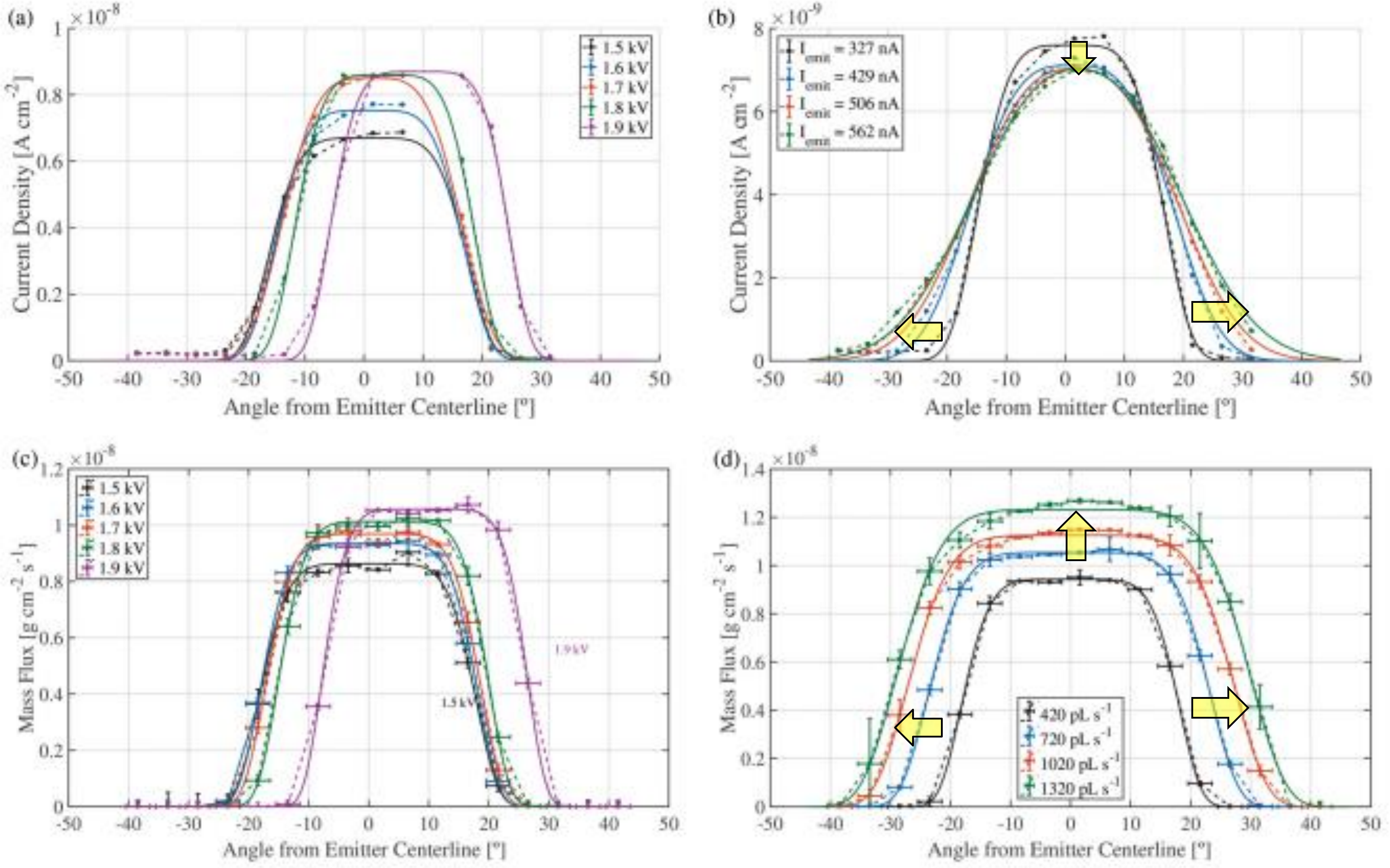


FIG. 3. Current density as a function of half angle for varying (a) extraction voltages (fixed flow rate of 420 pLs^{-1}) and (b) flow rates (constant voltage of 1.6 kV). Mass flux as a function of half angle for varying (c) extraction voltages (fixed flow rate of 420 pLs^{-1}) and (d) flow rates (constant voltage of 1.6 kV). All profiles shown with super-Gaussian fits. The trends of these fits with voltage and flow rates are shown in Fig. 5.

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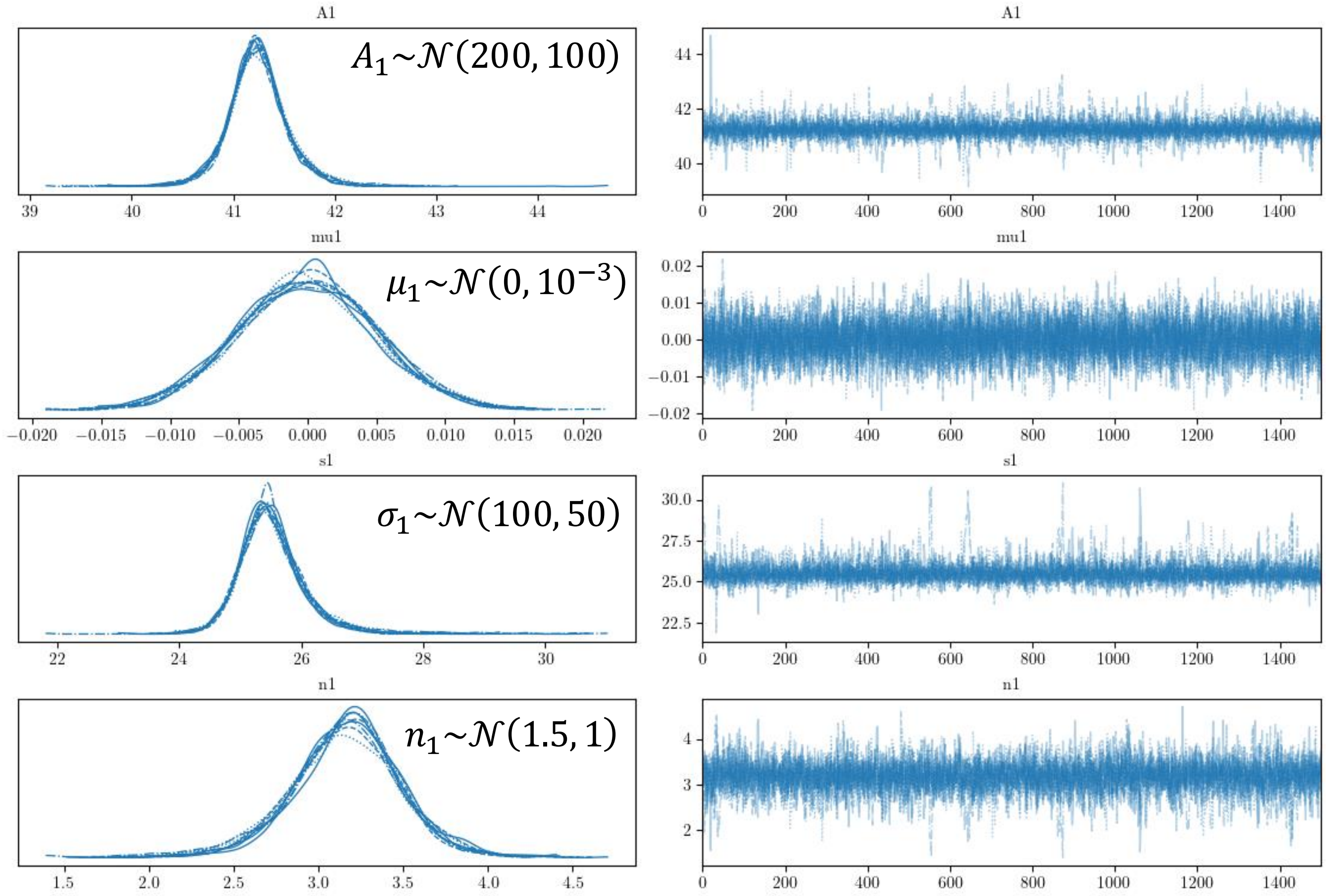
A - amplitude
σ – standard deviation
θ – plume angle
θ_t – plume tilt off central axis
n – sharpness (Gaussian for n=1)

A, σ, θ, θ_t, and n are physically-informed, unknown parameters that <u>inform</u> the function form of the following <u>likelihood</u> <u>function</u>.

Anirudh Thuppul, Peter L. Wright, Adam L. Collins, N. M. Uchizono, and Richard E. Wirz, “Mass Flux and Current Density Distributions of Electrospray Plumes,” *Journal of Applied Physics* (2020)

Results – Bayesian Inference



Posterior distributions (left) for unknown variables in PEPPER model—$f(\gamma_i)$ and "trace" plot (right) of all, 1500 drawn posterior distribution samples.

Bayes' Theorem
X, hypothesis X
Y, data
I, implicit model assumptions

$$prob(X|Y,I) = \frac{prob(Y|X,I) \cdot prob(X|I)}{prob(Y|I)}$$

Prior Distributions

$A_1 \sim \mathcal{N}(200, 100)$; $\mu_1 \sim \mathcal{N}(0, 10^{-3})$;
$\sigma_1 \sim \mathcal{N}(100, 50)$; $n_1 \sim \mathcal{N}(1.5, 1)$

Likelihood Function

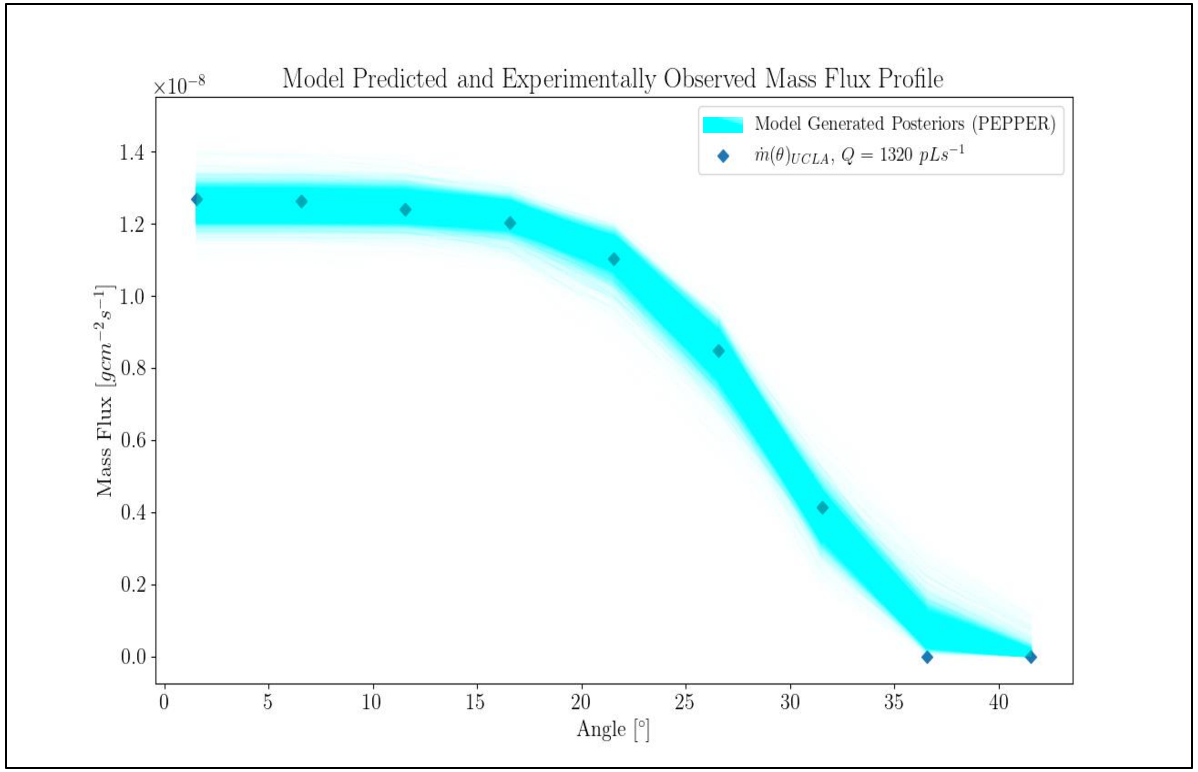
$$prob(\dot{m}(\theta)_{UCLA}|\gamma_i, I) = \prod_i^N prob(\dot{m}(\theta)_i|\gamma_i, I)$$

$$f(\theta_f) = \mathbb{M}(\theta_i, \boldsymbol{f}(\boldsymbol{\gamma_i}), V_{electrode}) \rightarrow \dot{m}(\theta)$$

$$f(\gamma_i) = \boldsymbol{A_1} \exp\left(-\frac{(\gamma_i - \boldsymbol{\mu_1})^2}{2\boldsymbol{\sigma_1}^2}\right)^{\boldsymbol{n_1}}$$

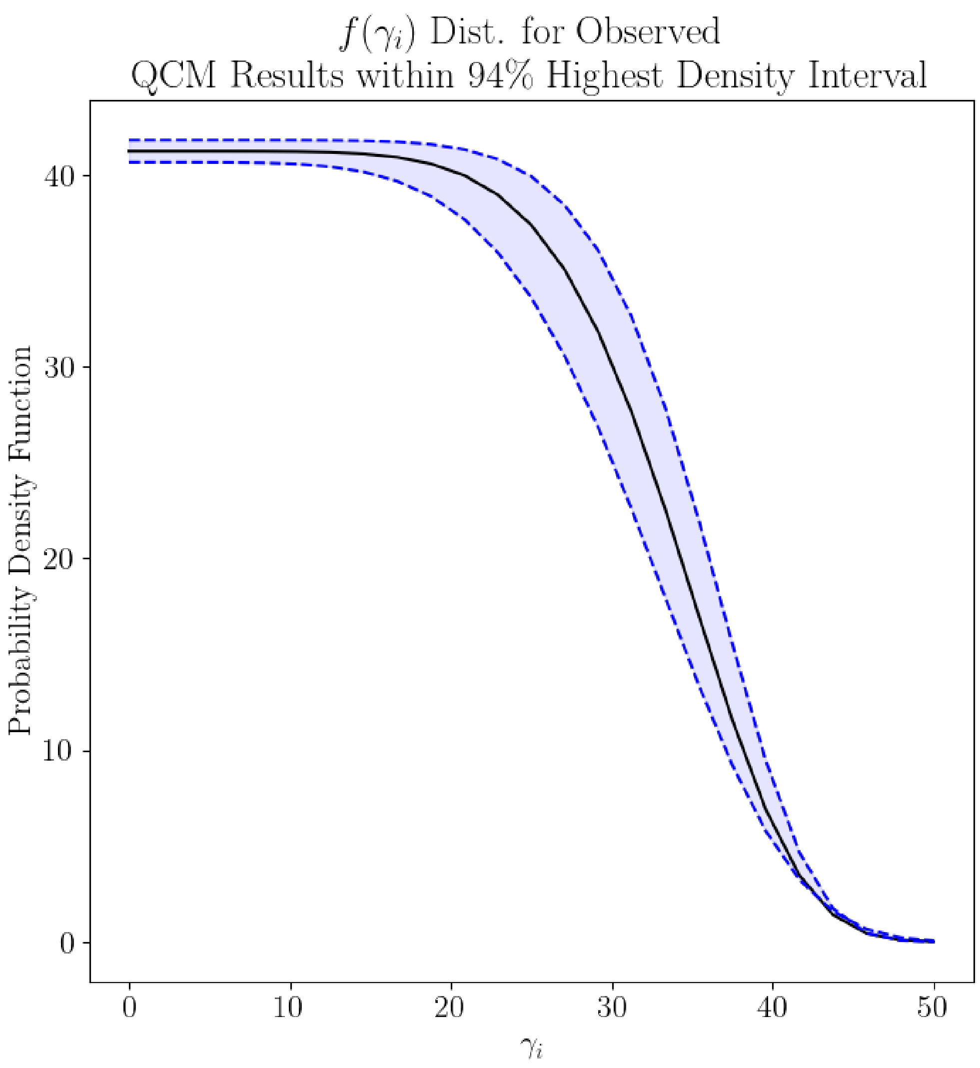
PEPPER – Bayesian Inference Results

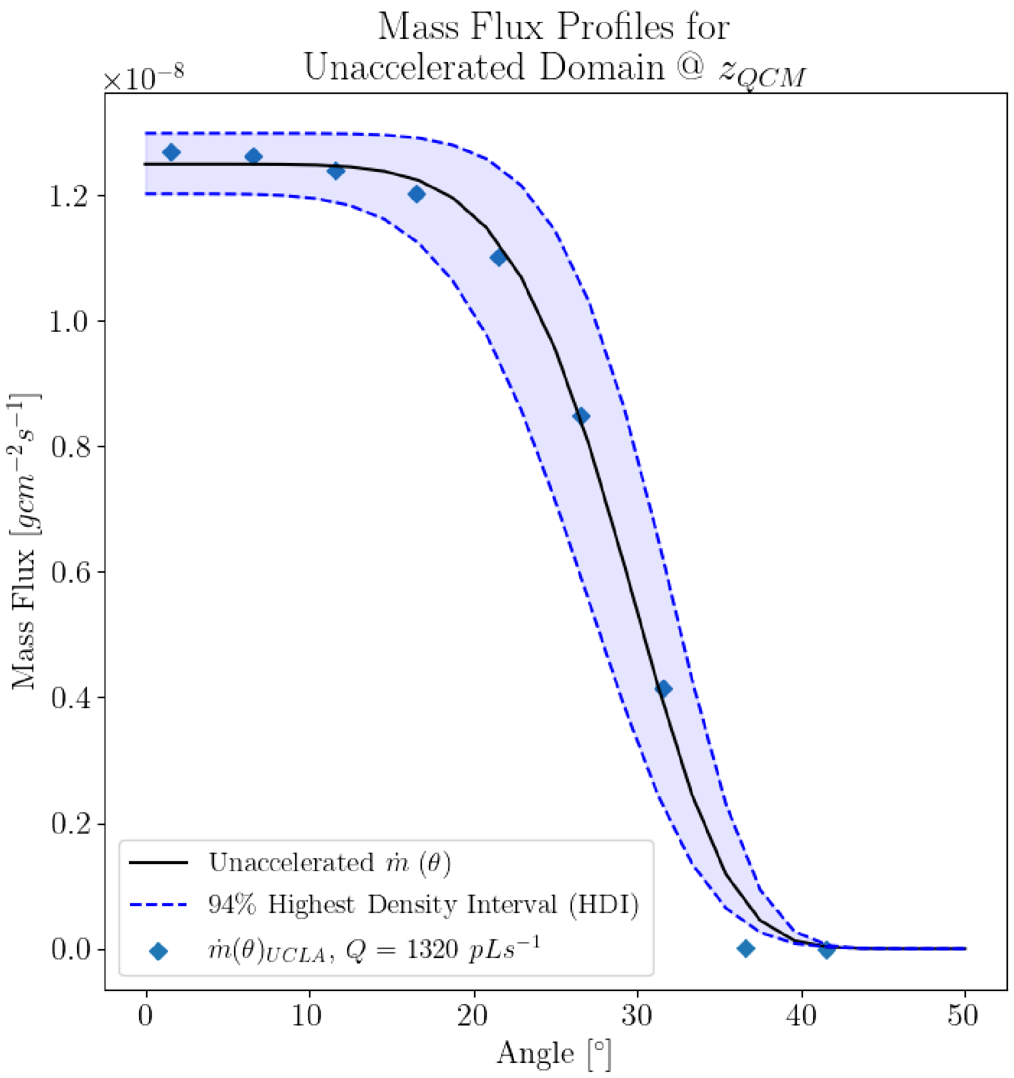
Unknown Parameter	Mean	Std. Deviation
A_1	41.246	0.306
μ_1	0.000	0.005
σ_1	25.533	0.585
n_1	3.158	0.330



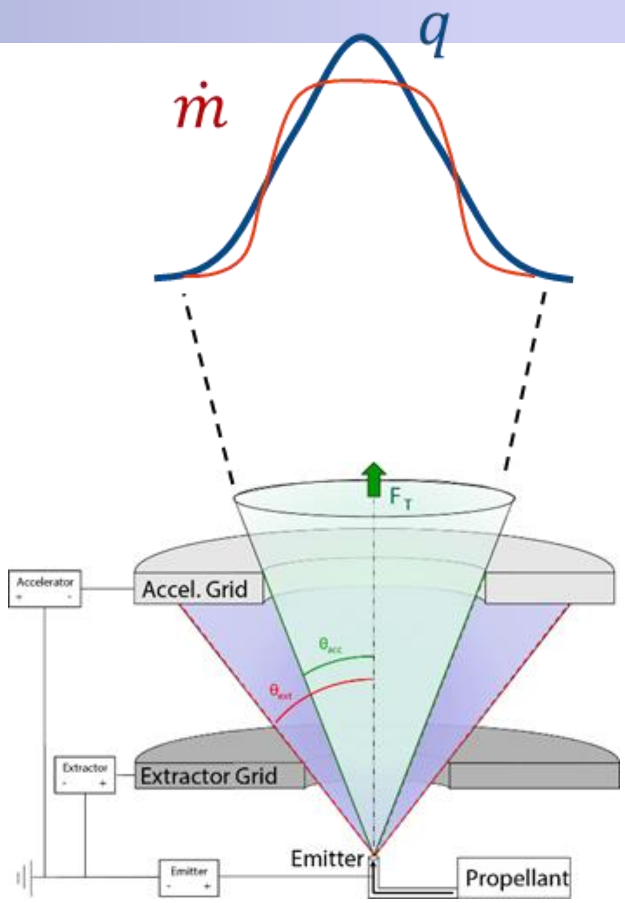
Complete mass flux profile for unaccelerated domain based on sampled posterior distributions.

PEPPER – Bayesian Inference Results





Conclusions



Research Objective: Determine initial conditions near emission site to explain observed Super-Gaussian plume profiles

- Data-driven modeling approach applied surrogate model and Bayesian inference to determine quantify unknown initial condition parameters
- Super-Gaussian distributions in initial emission angles result in downstream mass flux profiles observed experimentally
- Regions of higher uncertainty inform desirable experimental data points

Next Steps:

- Compare accelerated and unaccelerated electrospray domains
- Compare predicted charge density profiles with mass flux
- Use $\dot{m}(\boldsymbol{\theta})$→ Lifetime

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Thank you!

BONUS SLIDE: Research Overview

Motivation:

- Technological need for **improved electrospray lifetime and performance** for future missions of interest.
- Scientific need to **clarify governing physics** in electrospray plume expansion.

Objective:

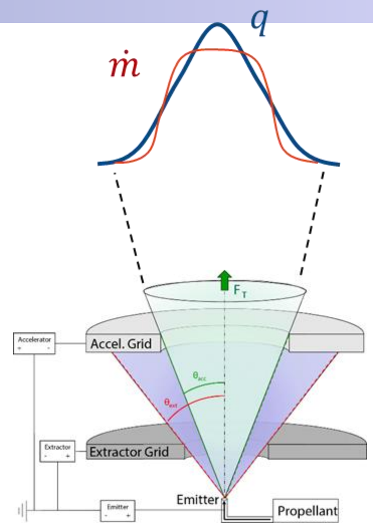
- Determine initial conditions near emission site to **explain observed Super-Gaussian plume profiles**

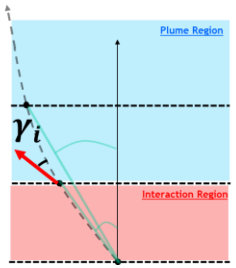
Hypotheses:

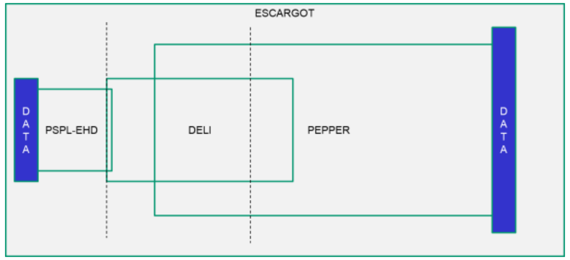
- Droplet dynamics in the **plume region are primarily governed by the external electric forces** generated by extractor and accelerator electrodes
- Grid impingement is most sensitive to the distribution of **initial emission angles** of droplets entering the plume region domain

Approach:

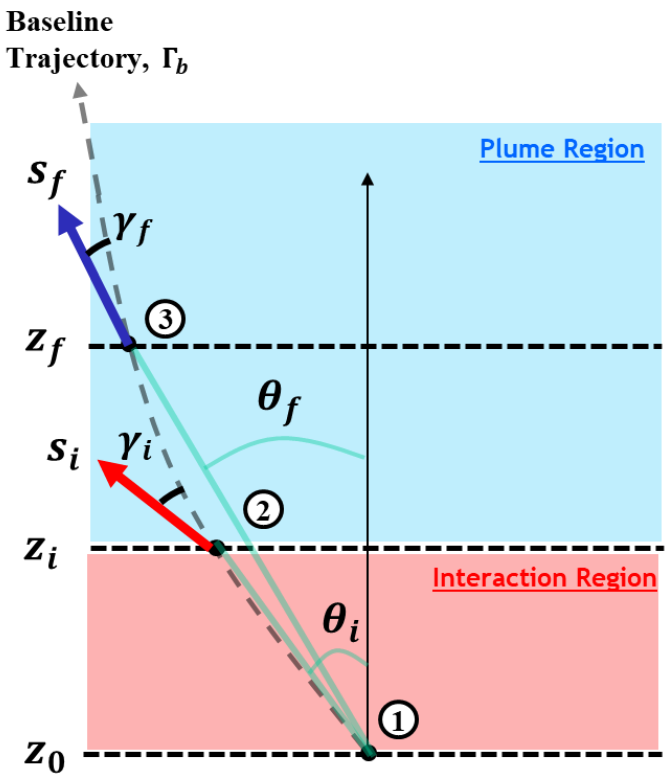
- Develop a **robust, data-driven modeling framework** for rapid lifetime and performance estimation
- Implement **surrogate modeling** techniques to reduce computational complexity of physics-based model
- Apply **Bayesian inference and statistical learning with available experimental results** in lieu of higher fidelity, direct numerical simulations







BONUS SLIDE: Plume Modeling Framework (Approach Overview)



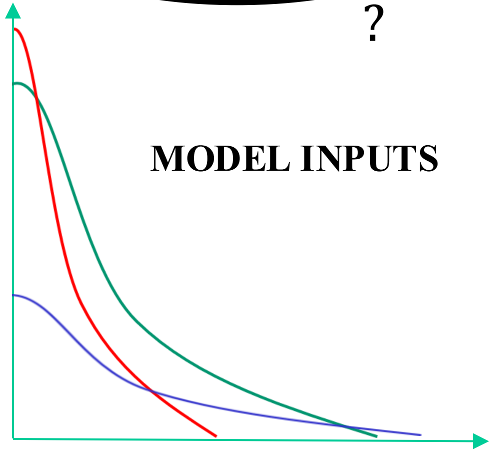
MODEL

$$\mathbb{M}\left(\frac{q}{m}, z_i, \theta_i, s_i, \gamma_i\right) \rightarrow \theta_f$$

1 2 3

$$f\left(\frac{KE_i}{q}\right), f(z_i, \theta_i), f(\gamma_i)$$

?



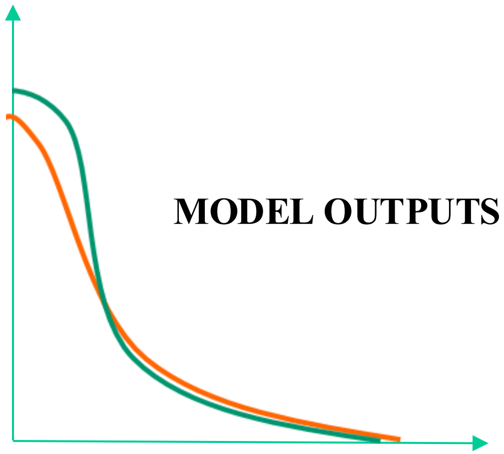
MODEL INPUTS

1 Forward Propagation

2 Backward Propagation

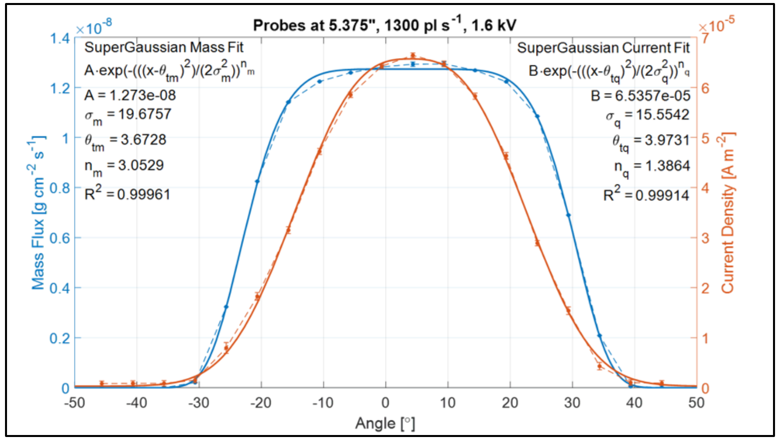
3 Prediction of plume profiles in arbitrary domain

$\dot{m}(\theta), j(\theta)$ @ $z = z_f$



MODEL OUTPUTS

Un-accelerated Profiles



Accelerated Profiles

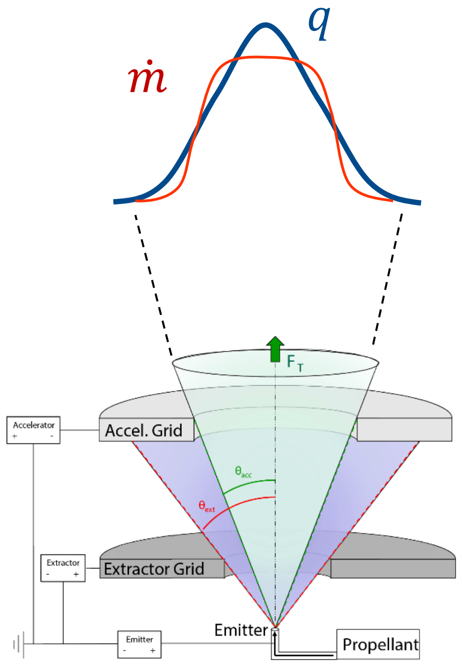
?

Mass and Charge Evolution in Electrospray Plumes for High Delta-V Thrusters

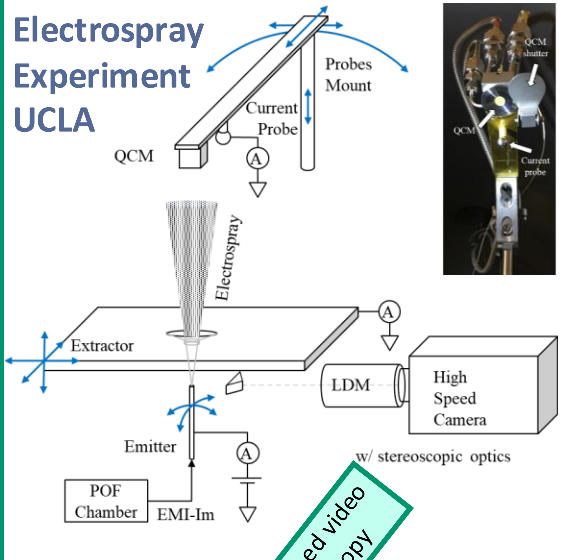
- **Project Objective:** Use advanced plume diagnostics and physics-based modeling to understand the mass and charge evolution in electrospray thruster plumes to predict performance and life for Air Force missions
- **PI:** Richard E. Wirz, UCLA, Plasma & Space Propulsion Laboratory

UCLA | PLASMA & SPACE PROPULSION LABORATORY

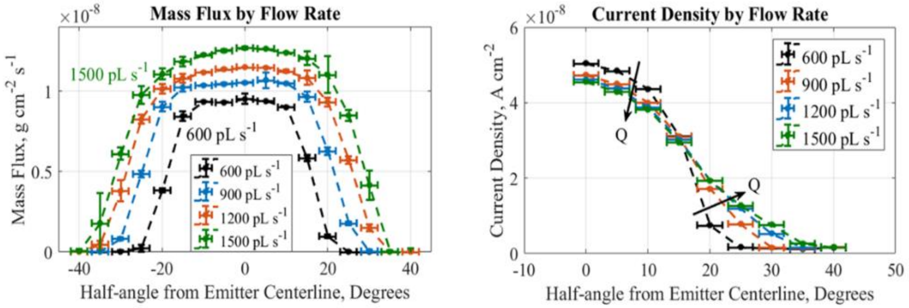
Challenge: Understanding mass ($\dot{m}$) and charge (q) evolution in electrospray plumes is critical for thruster life & performance



Electrospray Thruster



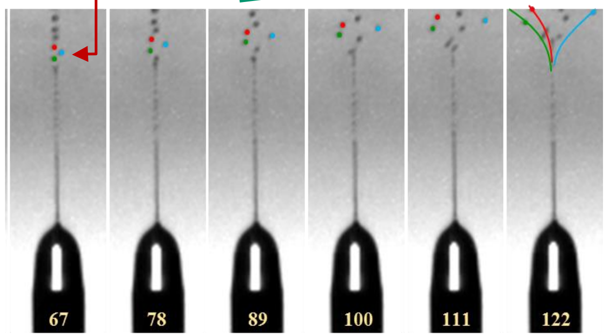
Plume diagnostics



UCLA and Air Force plume measurements show disparate evolution of mass and charge

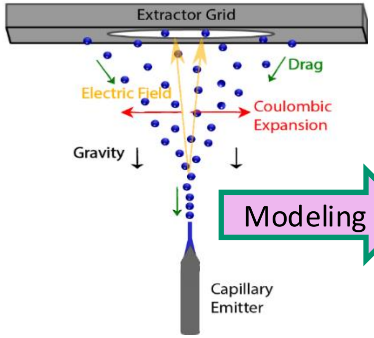
High-speed video microscopy

"traffic jam"



Time in μs

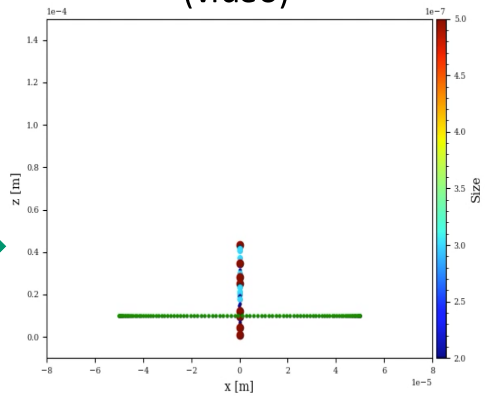
UCLA's high-speed videography and modeling implicate "traffic jam" collisions as primary cause of plume expansion



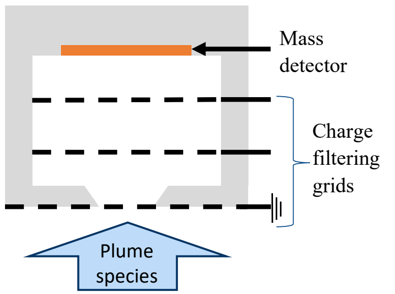
Modeling

Current Effort: UCLA is developing advanced diagnostics and physics-based modeling capabilities for determining electrospray thruster life & performance

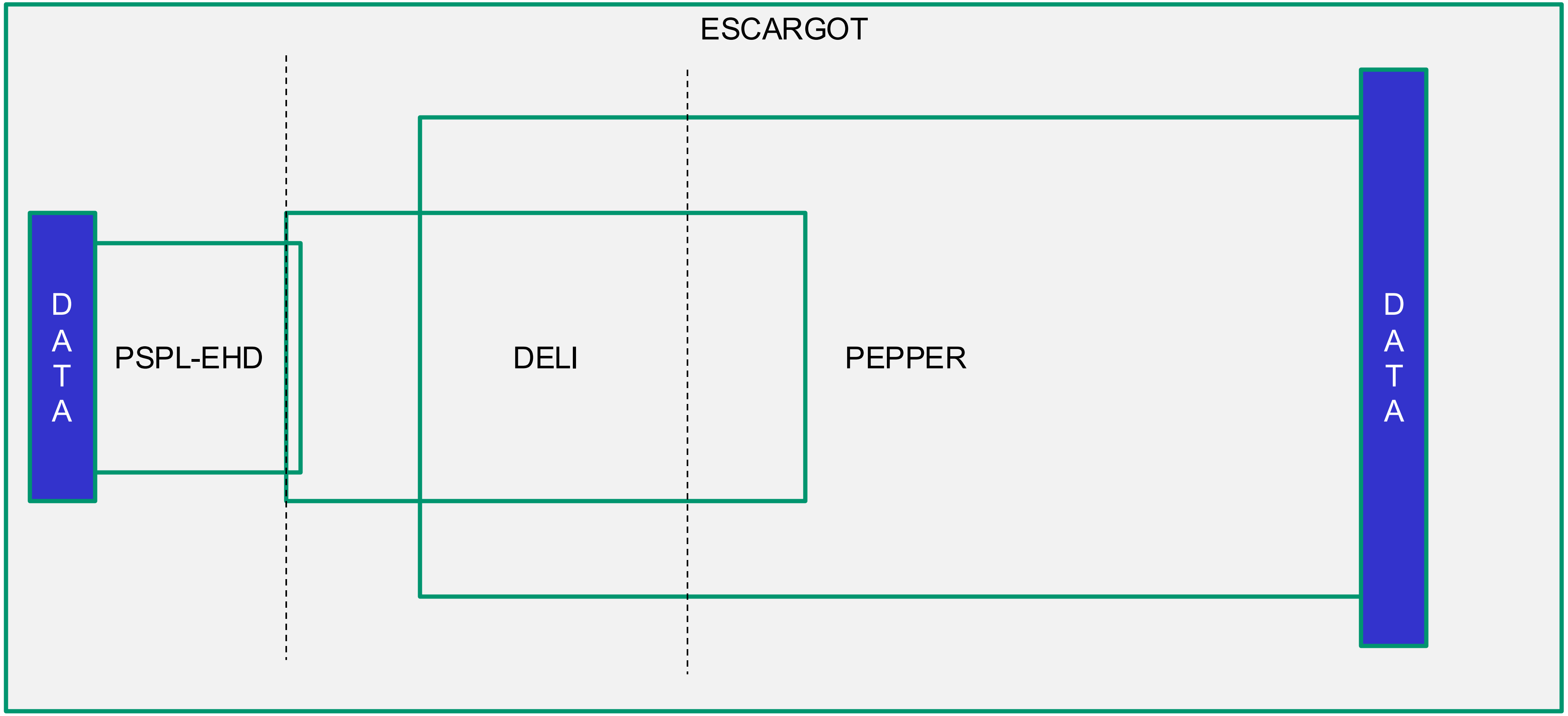
Physics-based plume modeling (video)



Precision charge & mass detector



BONUS SLIDE: Data-driven Modeling at the UCLA PSPL



Physics of electrosprays at UCLA PSPL investigated by computational models and experimental observations.

BONUS: Results – COMSOL Charged Particle Tracing

Electric Field Solver:

$$\boldsymbol{E} = -\nabla V$$

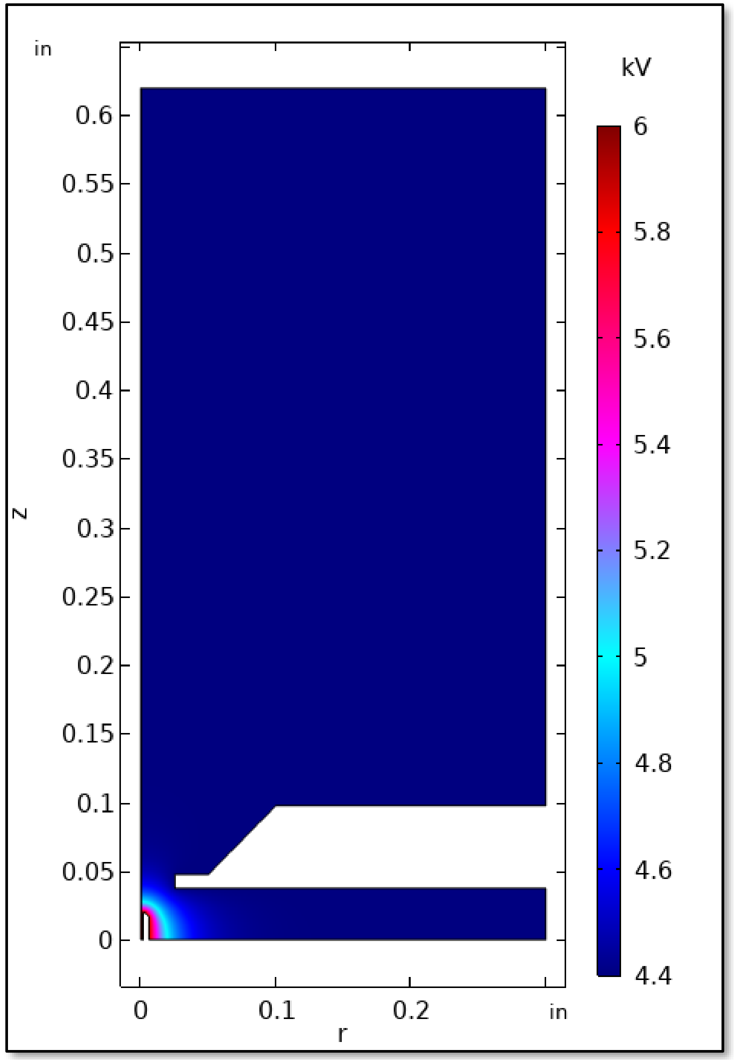
- Physics-controlled, "extremely fine", unstructured triangular mesh
- Bias Voltages set to: $V_{emit} = 6\ kV$; $V_{extr} = 4.4\ kV$; $V_{acc} = -1\ kV$; $V_{beam\ dump} = 0\ kV$
- Other Boundary Conditions:
  - Axial Symmetry at $r = 0$
  - Zero Charge elsewhere

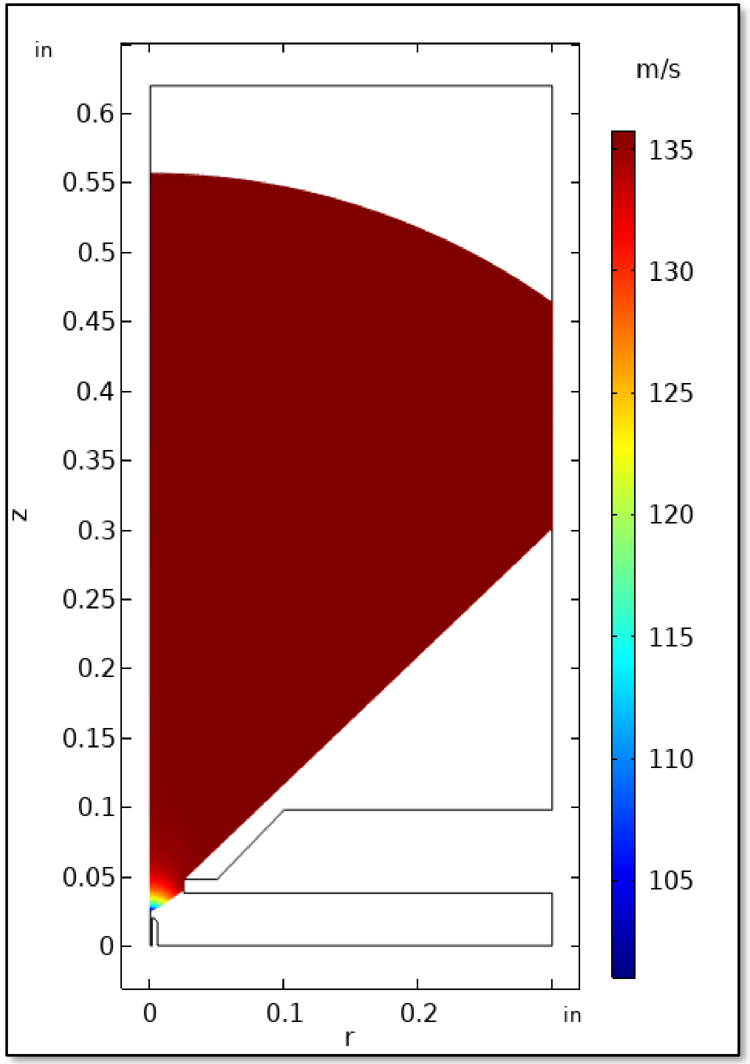
Charged Particle Tracing:

$$\frac{d(m_p \boldsymbol{v})}{dt} = \boldsymbol{F}_e = eZ\boldsymbol{E}$$

where e is elementary charge, m_p is the particle mass, and Z is the charge number.

- "Freeze" BCs at particle outlet (i.e. domain exit)
- Particle release conditions include initial kinetic energy, E_0, and initial particle direction, γ_i
  - Values for E_0 set to keep $\frac{KE}{q}$ constant at $\sim 10^2\ V$ for EMIM [1, 2]





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BONUS: Results – Surrogate Modeling

<u>Goal</u>: By how much (relatively) does each input parameter, $\boldsymbol{\theta_i}, \boldsymbol{\gamma_i}$, and $\mathbf{V_{acc}}$, influence the output parameter, $\boldsymbol{\theta_f}$, in $\mathbb{M}_{\mathrm{PCE}}$: $\boldsymbol{\theta_i}, \boldsymbol{\gamma_i}, \mathbf{V_{acc}} \rightarrow \theta_f$?

The *variance* of any function (like $Y_{PCE} = \mathbb{M}(\mathbf{X})$ from before) is defined by:

$$\boxed{V[f(X)] = \mathbb{E}[f(X) - \mathbb{E}(f(X))]^2}$$

Suppose we have a function, $f(\boldsymbol{X})$, where $\mathrm{X} = \mathrm{X}_1, \mathrm{X}_2, \dots, X_i$ defines the set of independent random variables for some $i \in [0, p]$. We can find the importance of each X_i on $V[f(\boldsymbol{X})]$ by decomposing $f(\boldsymbol{X})$ into 2^p orthogonal functional terms of increasing dimension [1]:

$$f(\boldsymbol{X}) = f_0 + \sum_{i=1}^{p} f_i(X_i) + \cdots + f_{1,2,\dots,n}(X_1, \dots, X_p)$$

*ANOVA decomposition specifically for PCEs [2]

Then, the total variance of $f(\boldsymbol{X})$ follows, where V is the *total variance* and V_i is the *partial variance* contribution of X_i, and $V_u(u \in [1, \dots, p])$ is the *interactive variance* contribution of X_u (one can think of it as a conditional variance, where $V_u = V(f(X_i)|X_i)$):

$$V = \sum_{i=1}^{p} V_i + \sum_{1 \le i \le j \le p} V_{ij} + \cdots + V_{1,2,\dots,p}$$

The result is a first-order sensitivity index. We can now conduct a quantitative <u>sensitivity analysis</u> of our physical parameters using <u>variance-based Sobol indices</u>.

$$S_u = \frac{V_u}{V}, \text{ where } S_u \le 1$$

[1] Sobol IM (1993) Sensitivity estimates for nonlinear mathematical models. Math model comput exp 1(1):112–118
[2] Sudret B (2008) Global sensitivity analysis using polynomial chaos expansions. Reliab Eng Syst Saf 93(7):964–979

FIGURE: PEPPER – Model Diagram