A Bayesian Data-driven Model for Quantifying Electrospray Lifetime

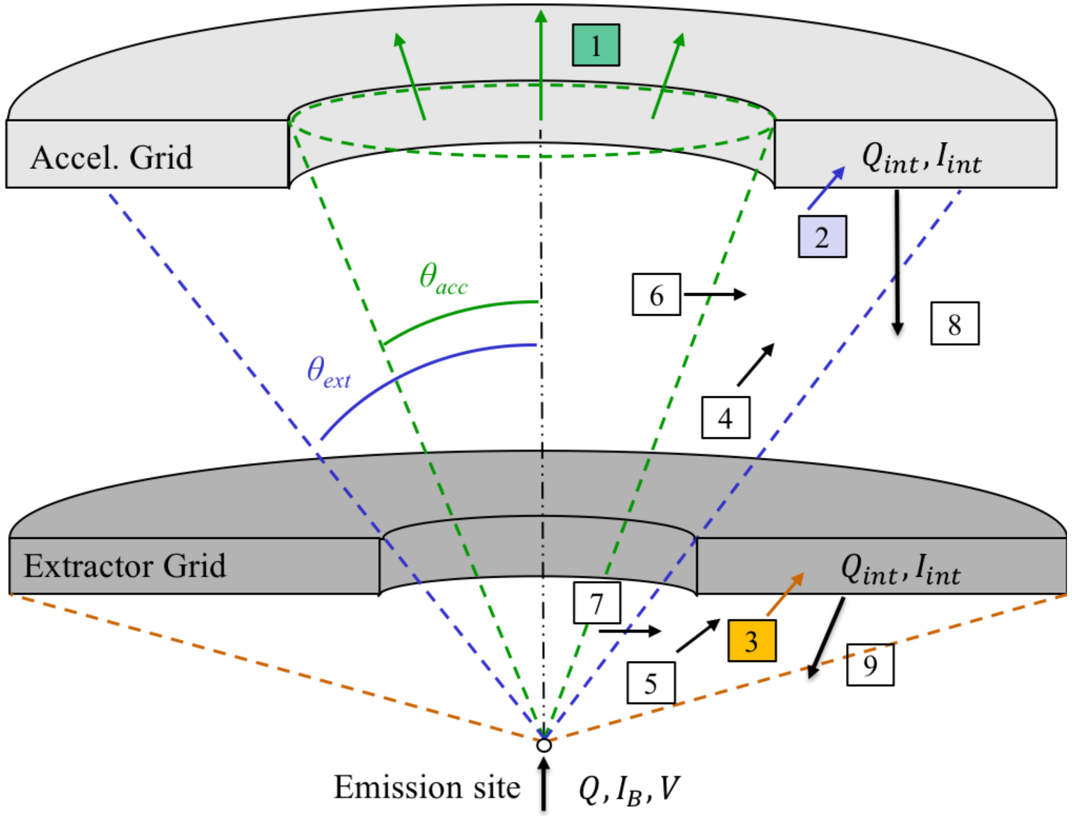
IEPC-2022-230

Shehan Parmar, Dr. Adam L. Collins, and
Prof. Richard E. Wirz
UCLA Plasma and Space Propulsion Laboratory
University of California, Los Angeles

International Electric Propulsion Conference
Boston, MA
20 June 2022

UCLA
PLASMA, ENERGY, & SPACE PROPULSION
LABORATORY

Background

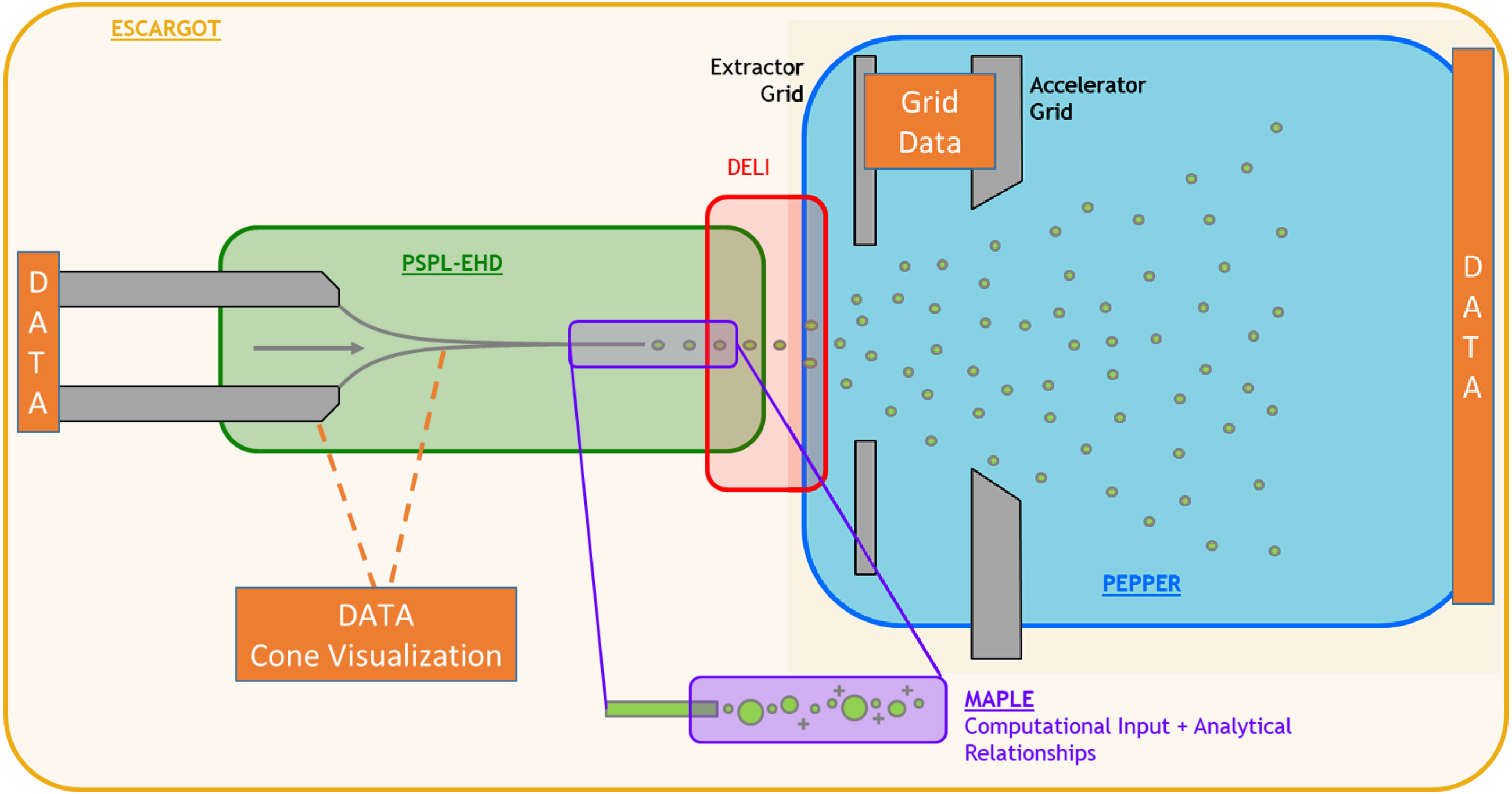


- **1** → T, Thrust from electrospray emission through accelerator grid
- **2** → $\dot{m}_{acc}$, Propellant mass flux toward accelerator grid
- **3** → $\dot{m}_{ext}$, Propellant mass flux toward extractor grid

- Overspray is a primary life-limiting failure mechanism for electrospray thrusters
- Minimizing mass flux 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

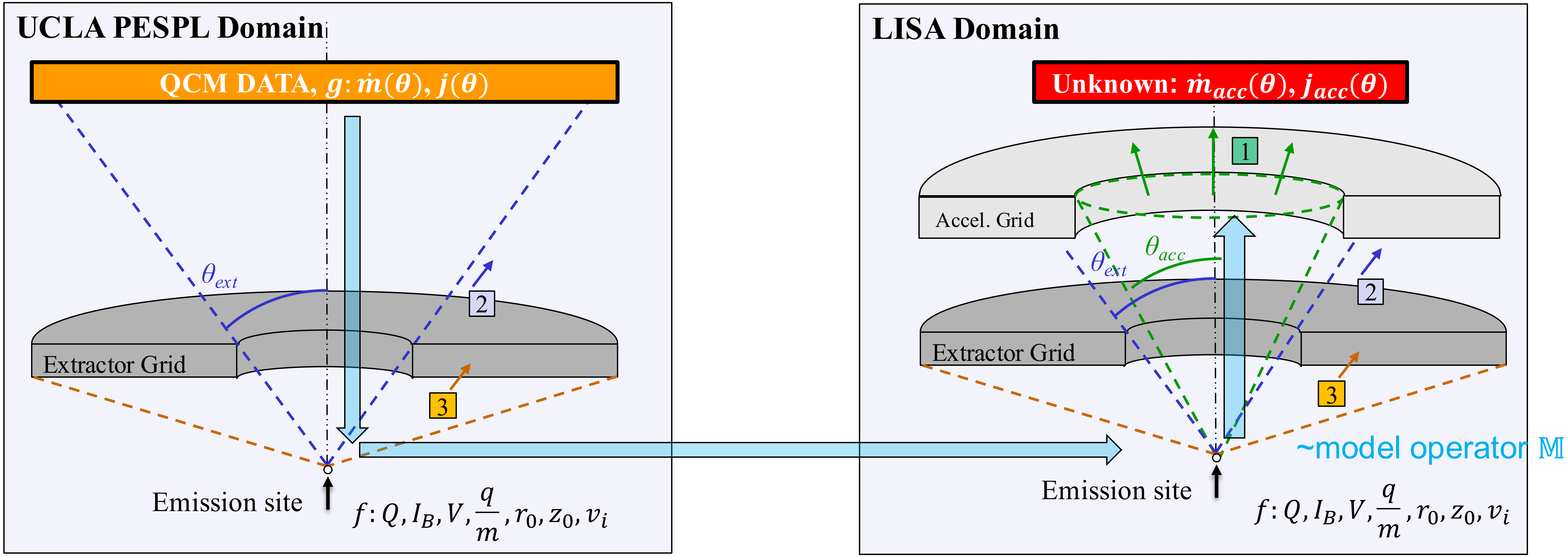
UCLA PESPL Experimental and Computational Domain



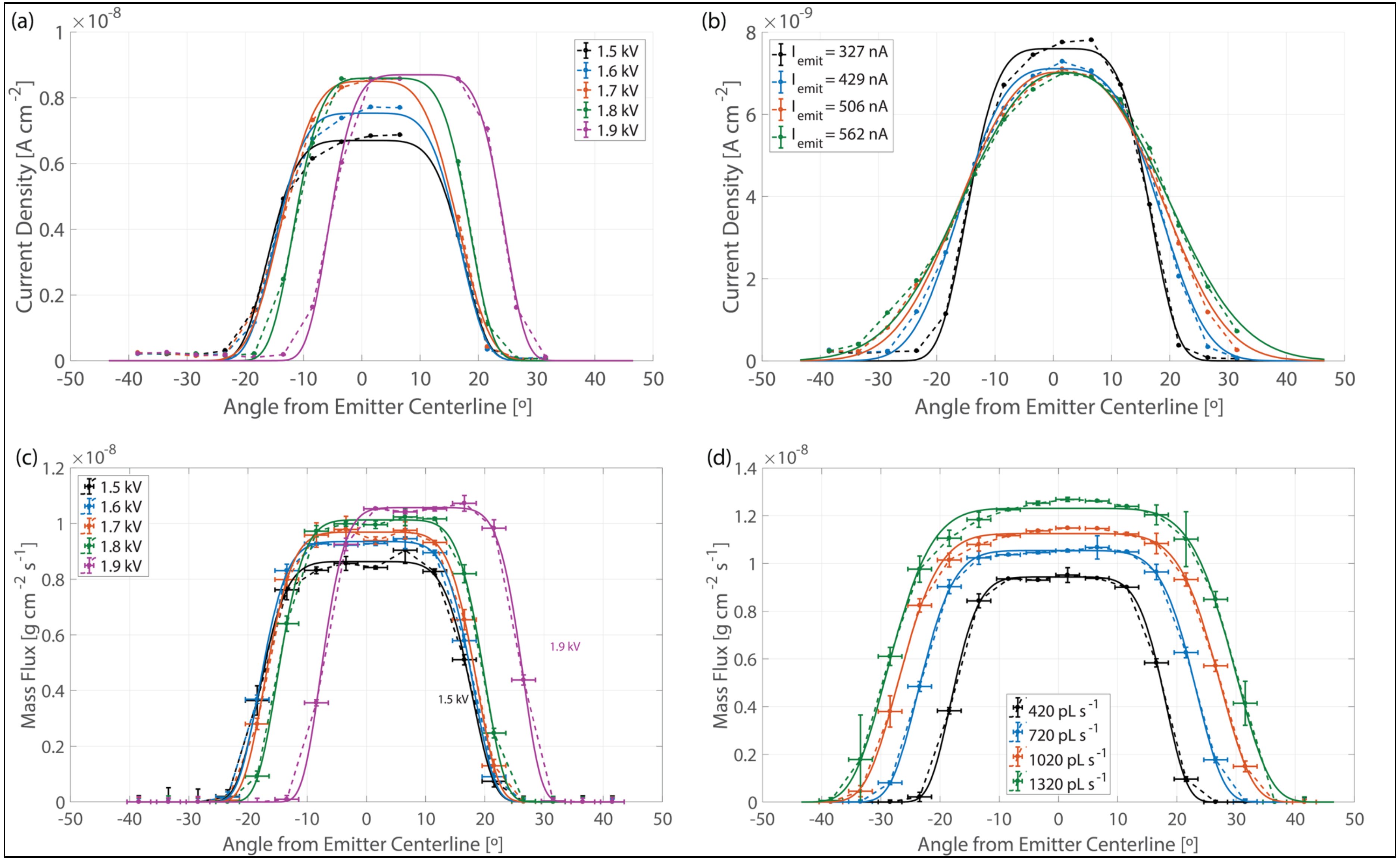
Inverse Problem Formulation

Objective: Given measured data $g \in Y$ with uncertainty $e \in Y$ and forward model operator $\mathbb{M}: X \rightarrow Y$, reconstruct model parameters $f \in X$ such that

$$g = \mathbb{M}(f) + e.$$



Electrospray Plume Profiles



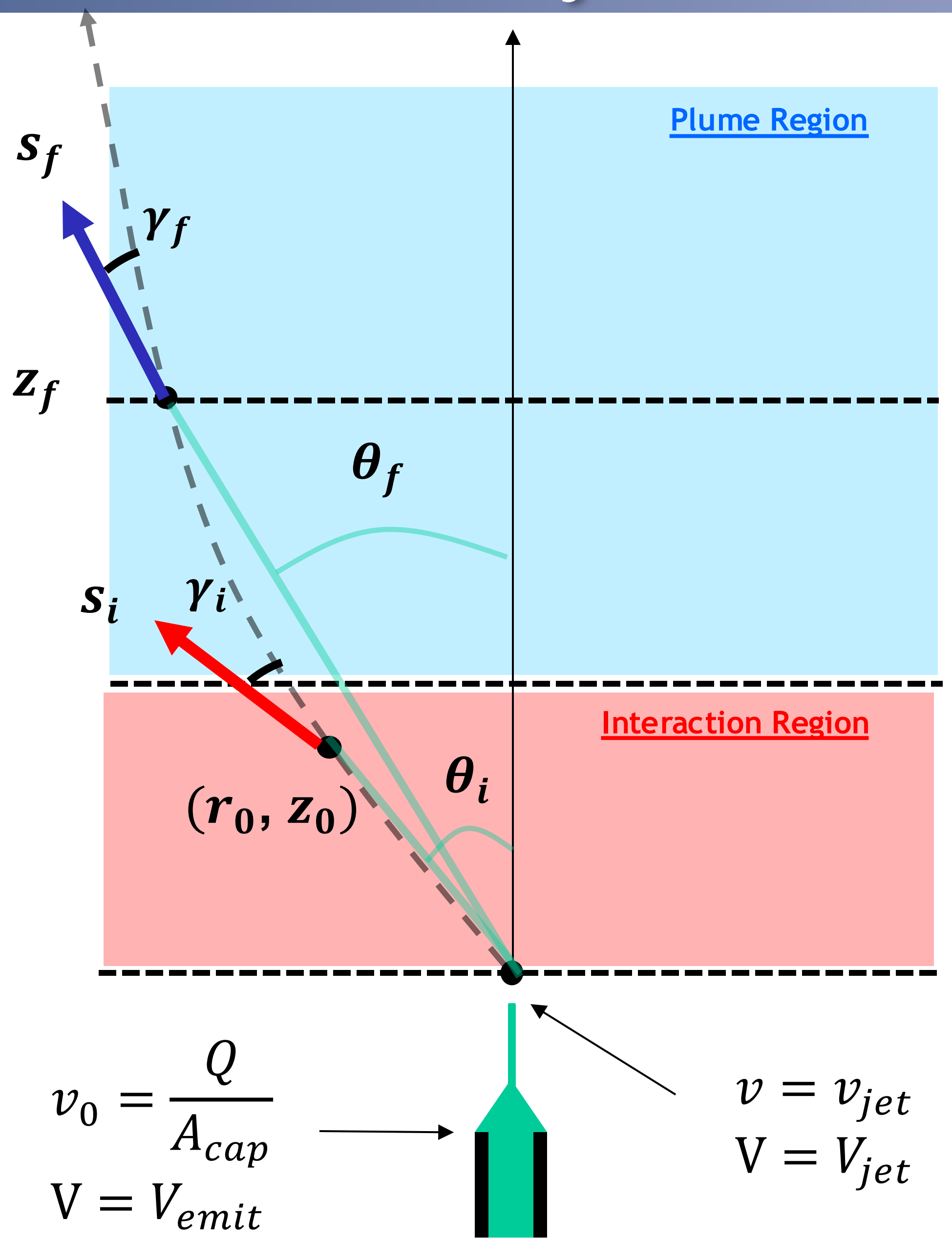
Super-Gaussian Form:

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

A - amplitude
σ – standard deviation
θ – plume angle
n – sharpness (n=1 for Gaussian)

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* (2021)

Model Geometry



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_0, z_0: 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:

$$\frac{KE}{q} = \frac{1}{2}\frac{m}{q}\vec{v}_i^2 = V_{jet} - V_{emit} = const$$

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

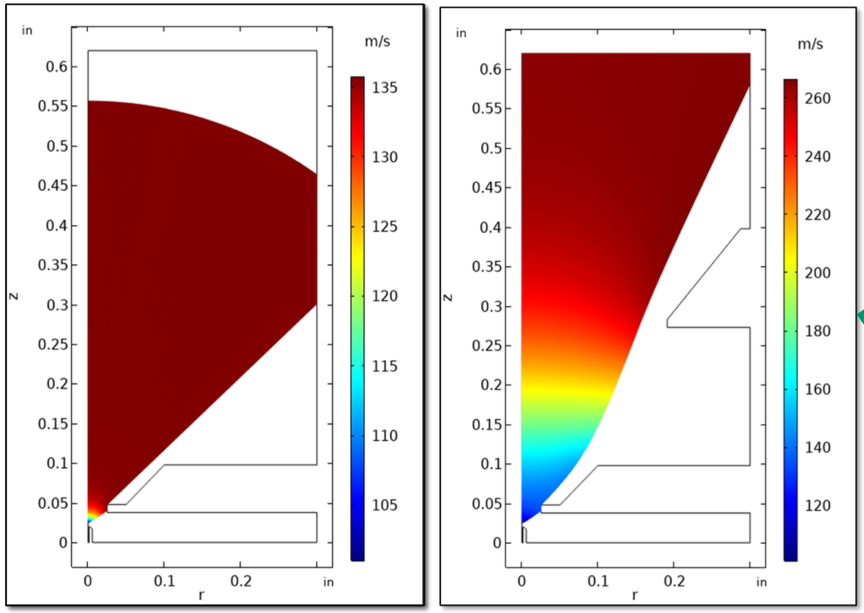
θ_i: initial position based on r_0, z_0
γ_i: initial emission angle
V_{extr}, V_{acc}, etc.: Geometry/Domain Specific inputs

Surrogate Modeling

$$\mathbb{M}(r,z) = \sum_{i,j}^{n} C_{ij} r^i z^j$$

Un-accelerated Domain

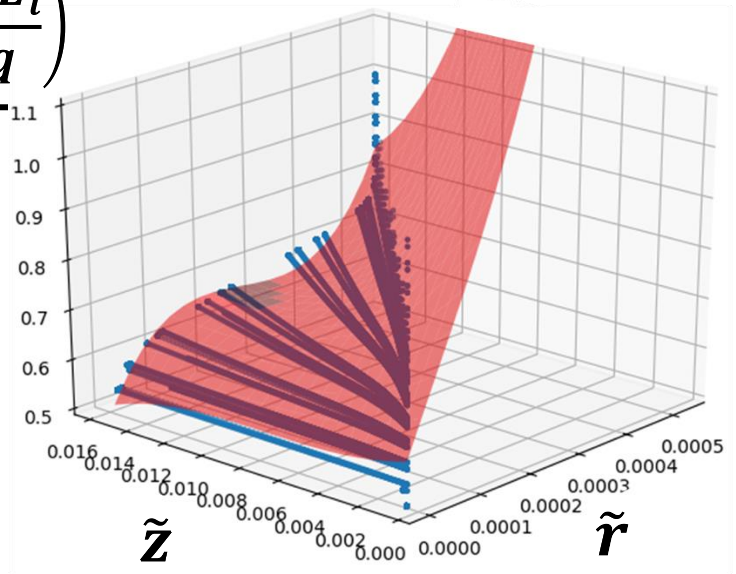
Accelerated Domain



1D Comparison of Accelerated vs. Non-Accelerated Grid Geometries

$$\mathbb{M}: \left(\frac{1}{2}\frac{m}{q}\right) \quad log\left(\frac{KE_i}{m}\right)$$

n	R^2
1	0.994
2	0.998
3	1.000

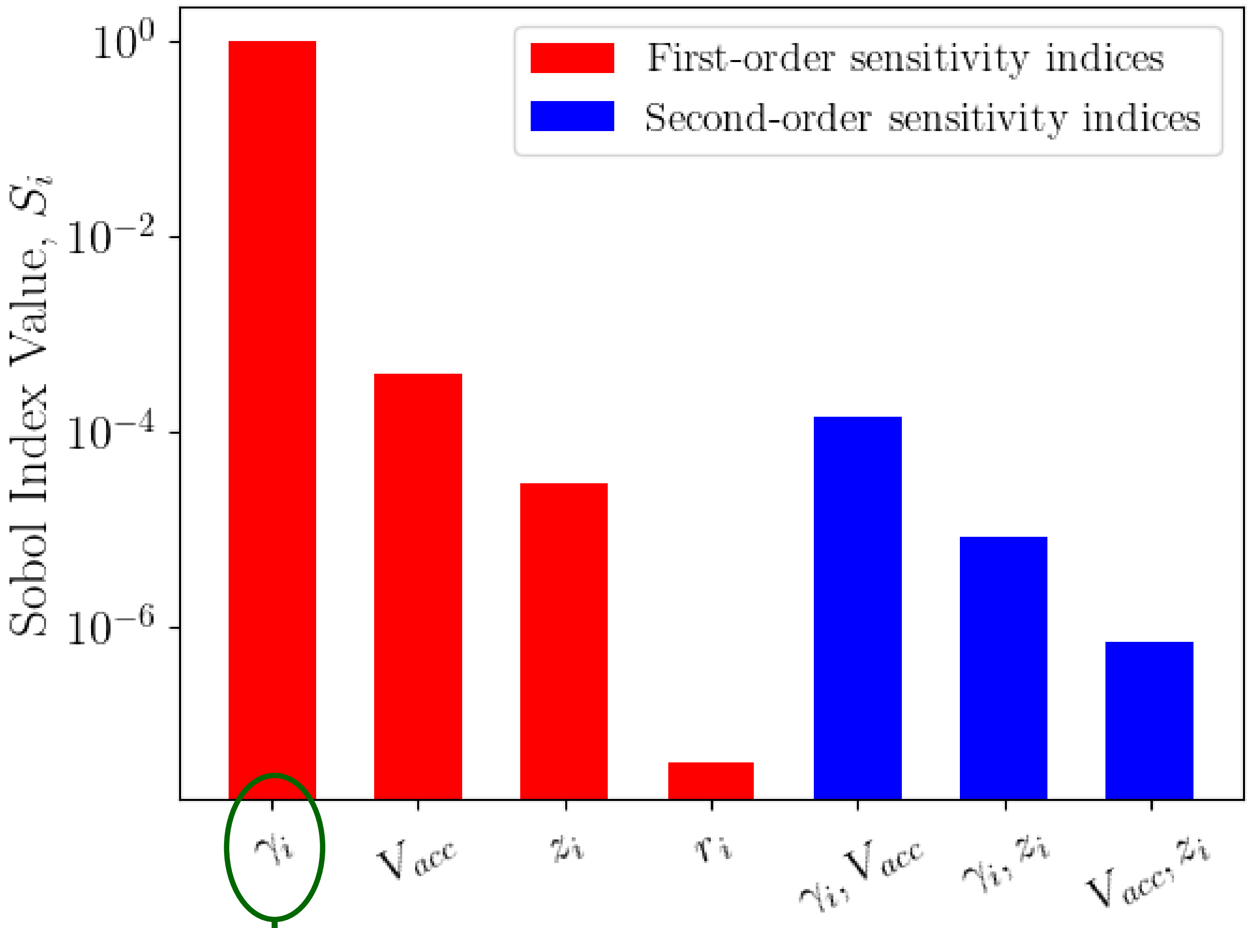


$$\mathbb{M}(\boldsymbol{X}) = \sum_{\alpha \in N^d} y_\alpha \Psi_\alpha(\boldsymbol{X})$$

$$\langle \Psi_\alpha, \Psi_\beta \rangle = 0$$

Previous Results – Sensitivity Analysis

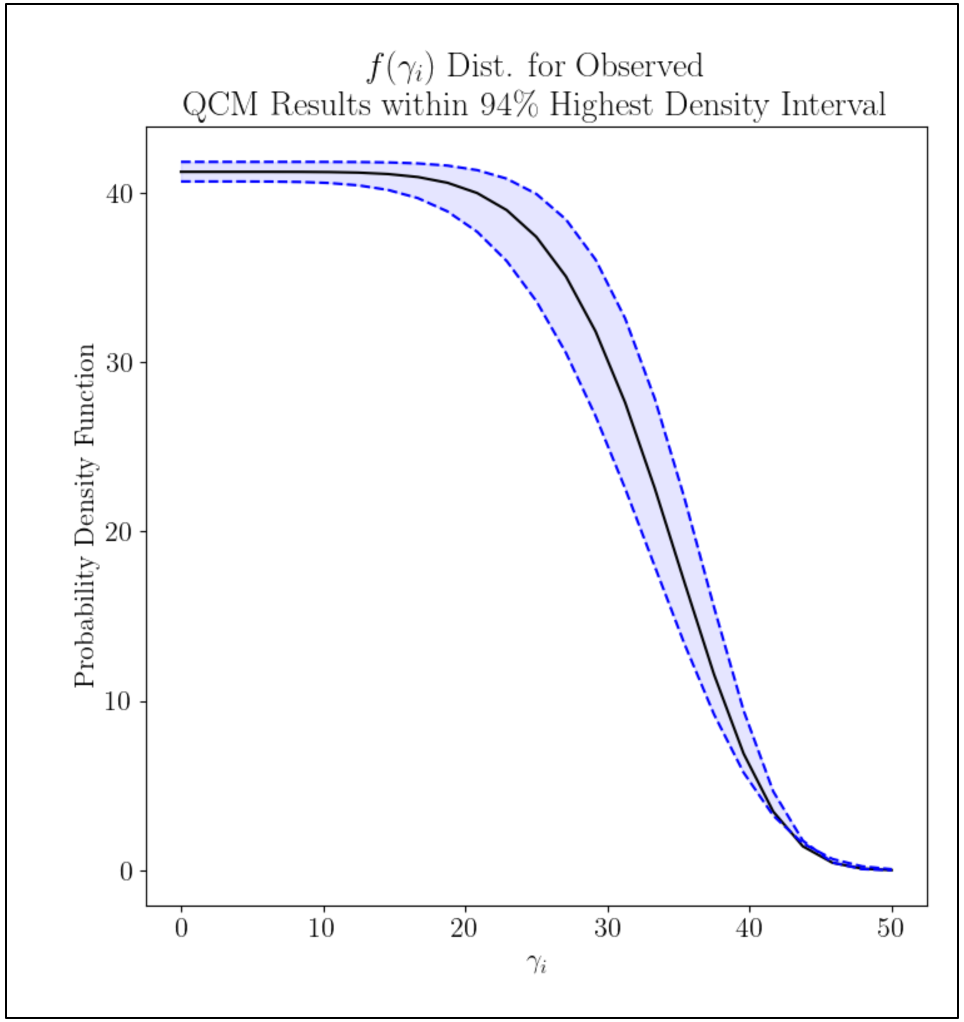
Goal: By how much (relatively) does each input parameter, $\boldsymbol{\theta_i}, \boldsymbol{\gamma_i}$, and $\mathbf{V_{acc}}$, influence the output parameter, $\boldsymbol{\theta_f}$, in $\mathbb{M}_{PCE}: \boldsymbol{\theta_i}, \boldsymbol{\gamma_i}, \mathbf{V_{acc}} \rightarrow \theta_f$?



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

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

Bayesian Inference – Results



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

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

Likelihood Function

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

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

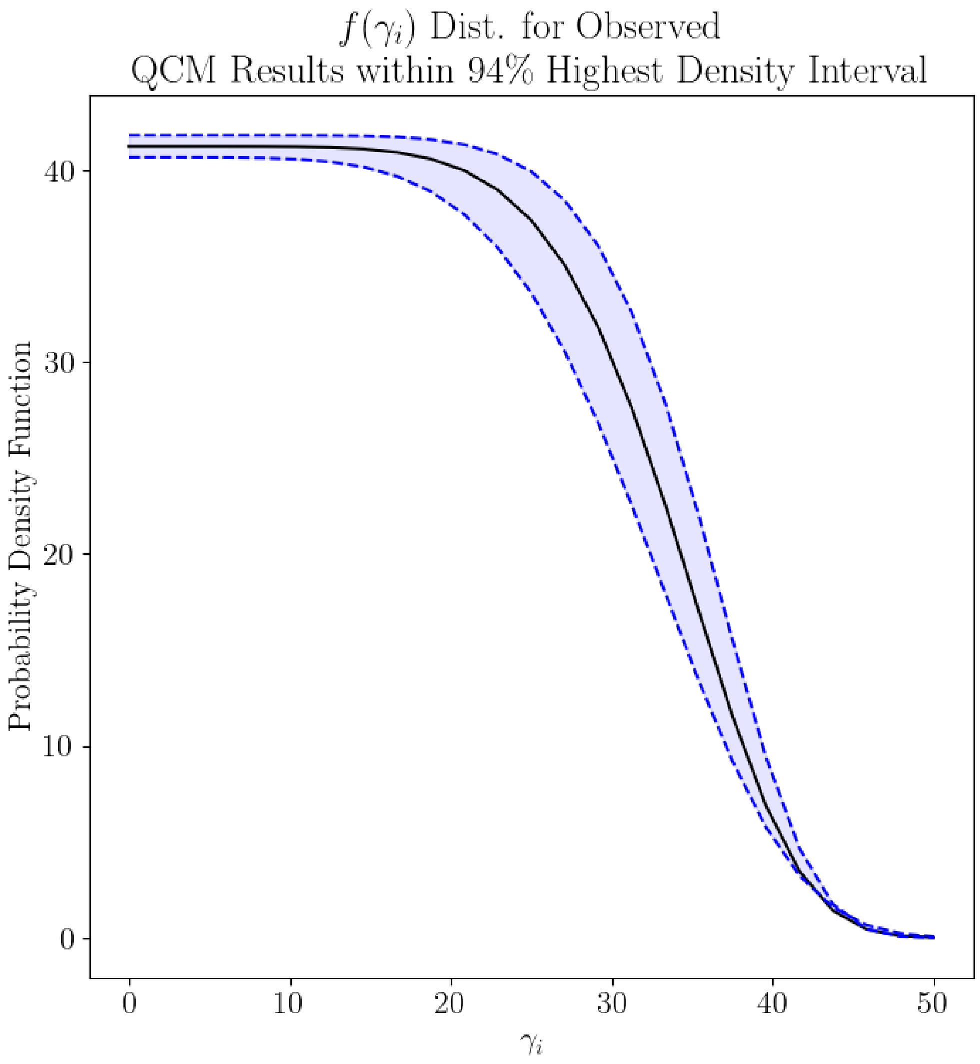
$$f(\gamma_i) = \boldsymbol{A_1} \exp\left(-\frac{(\gamma_i - \boldsymbol{\mu_1})^2}{2\boldsymbol{\sigma_1^2}}\right)^{\boldsymbol{n_1}}$$

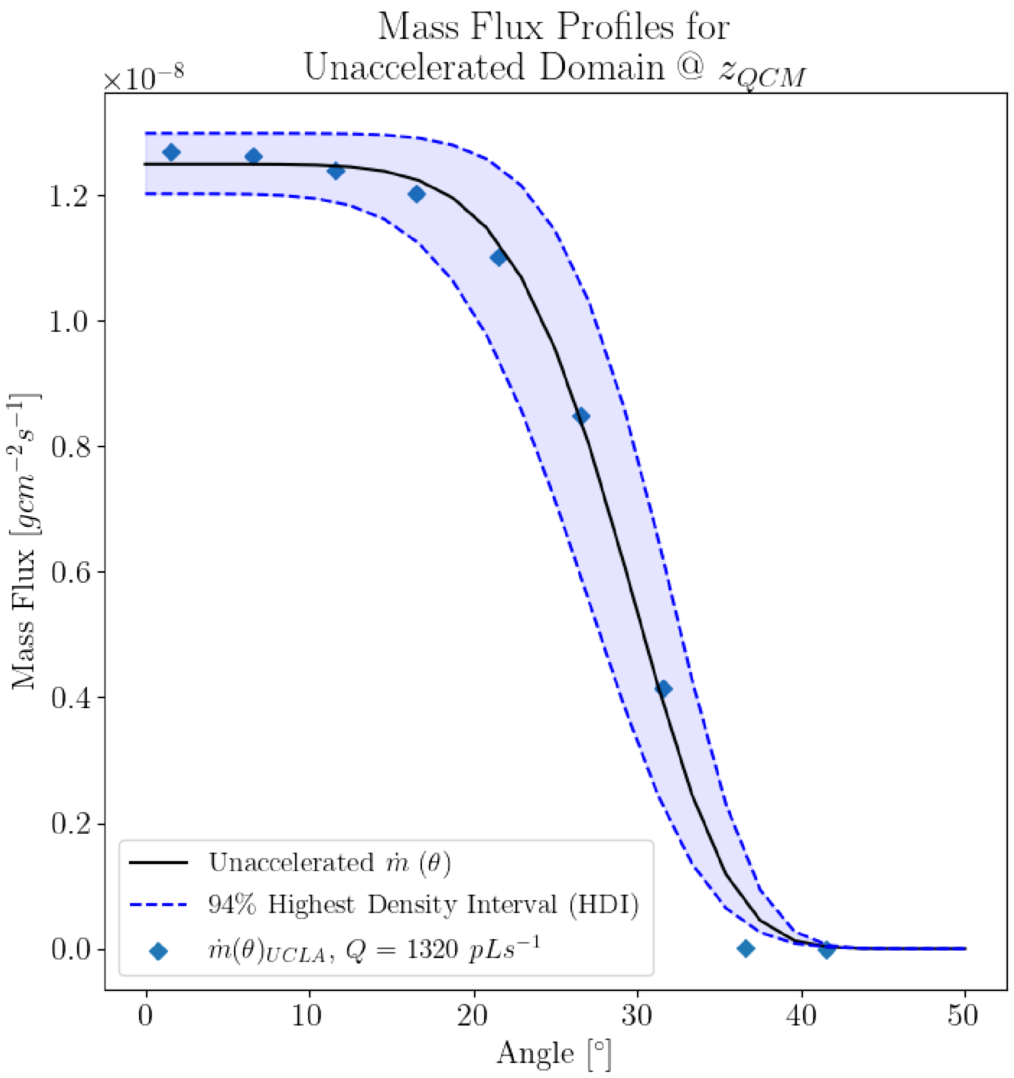
Prior Distributions

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

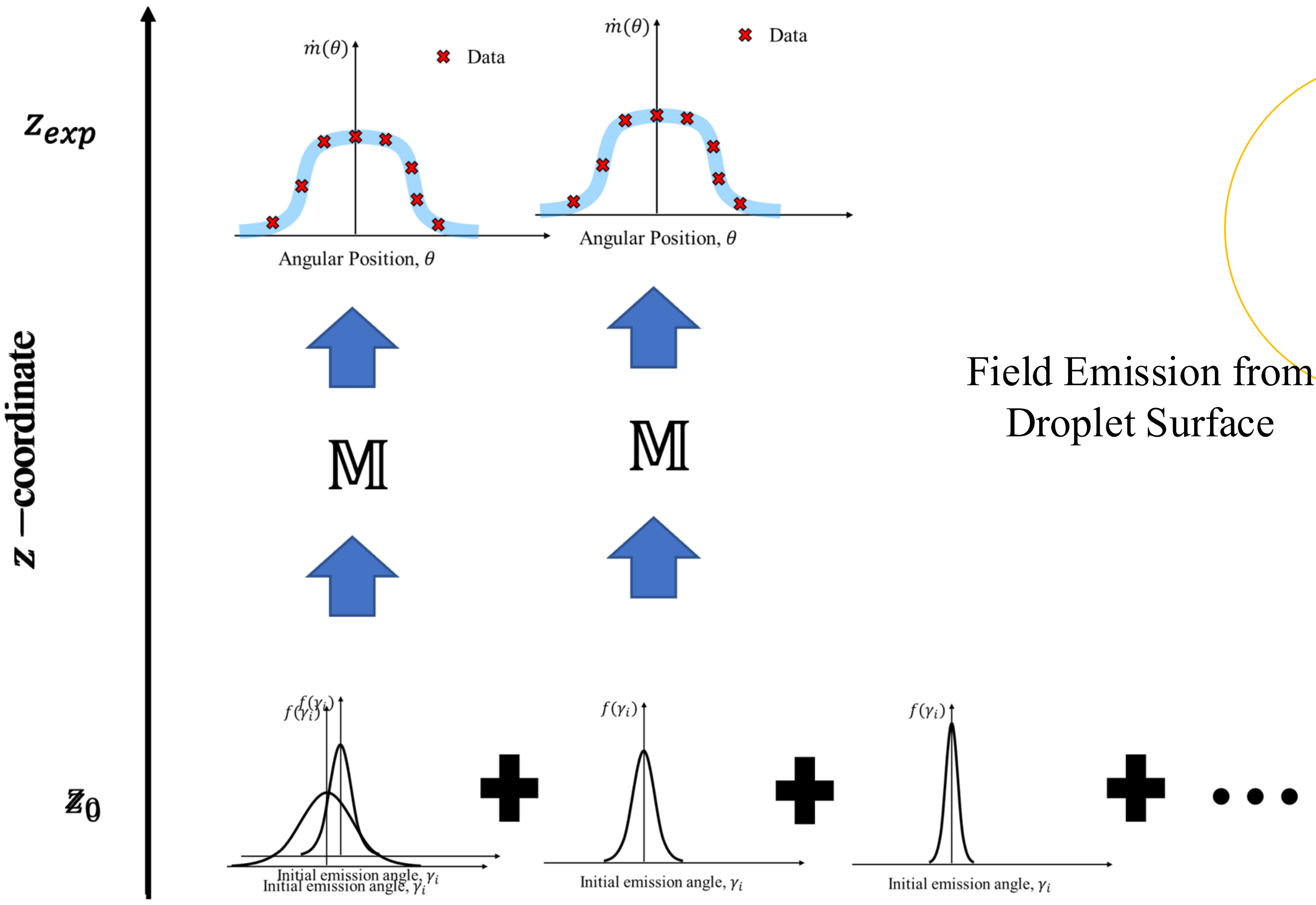
Results based on provided data sets (Thuppul et al., 2020) suggest **most probable functional form of γ_i** must also follow **Super-Gaussian shape**.

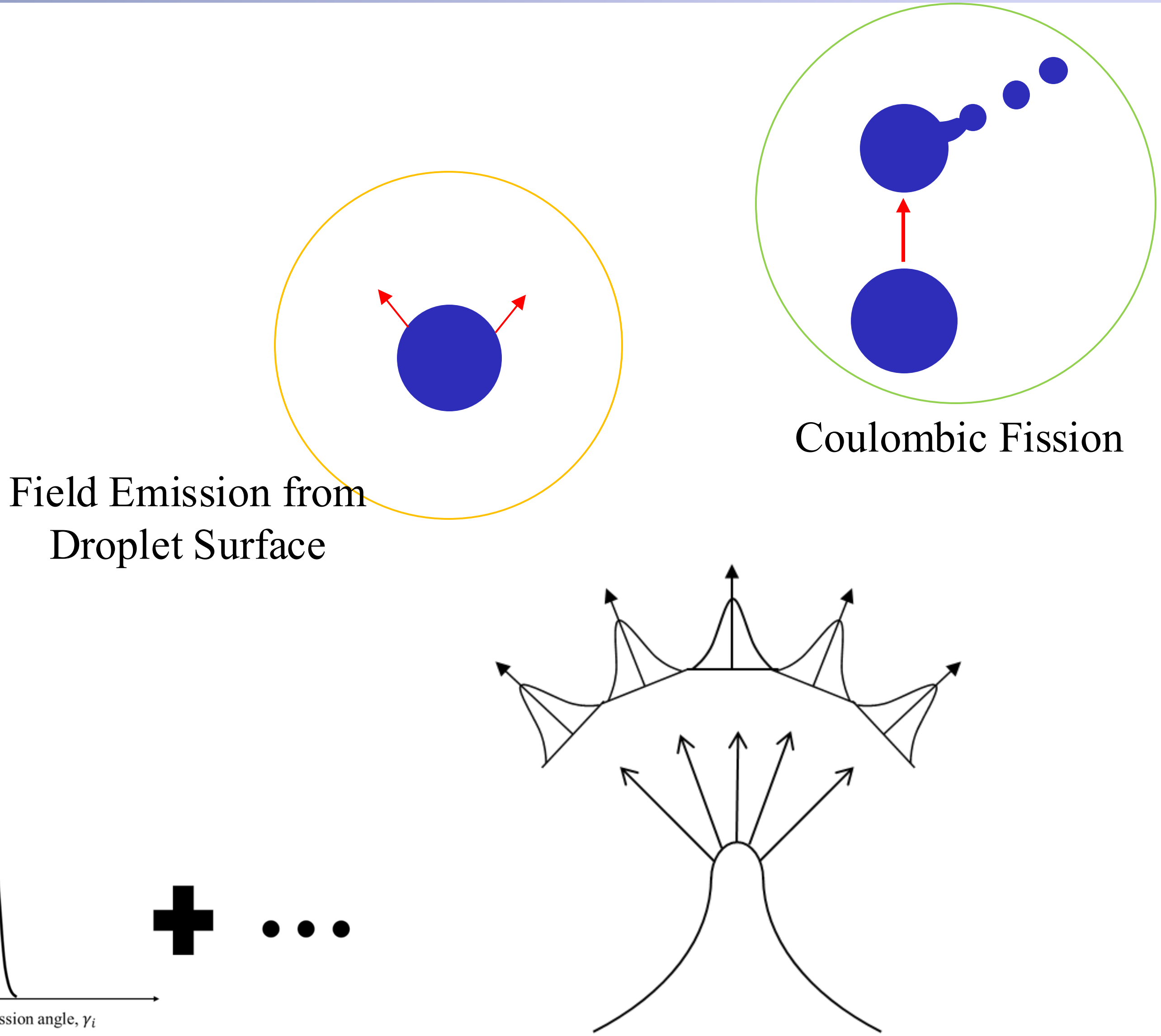
Bayesian Inference – Results



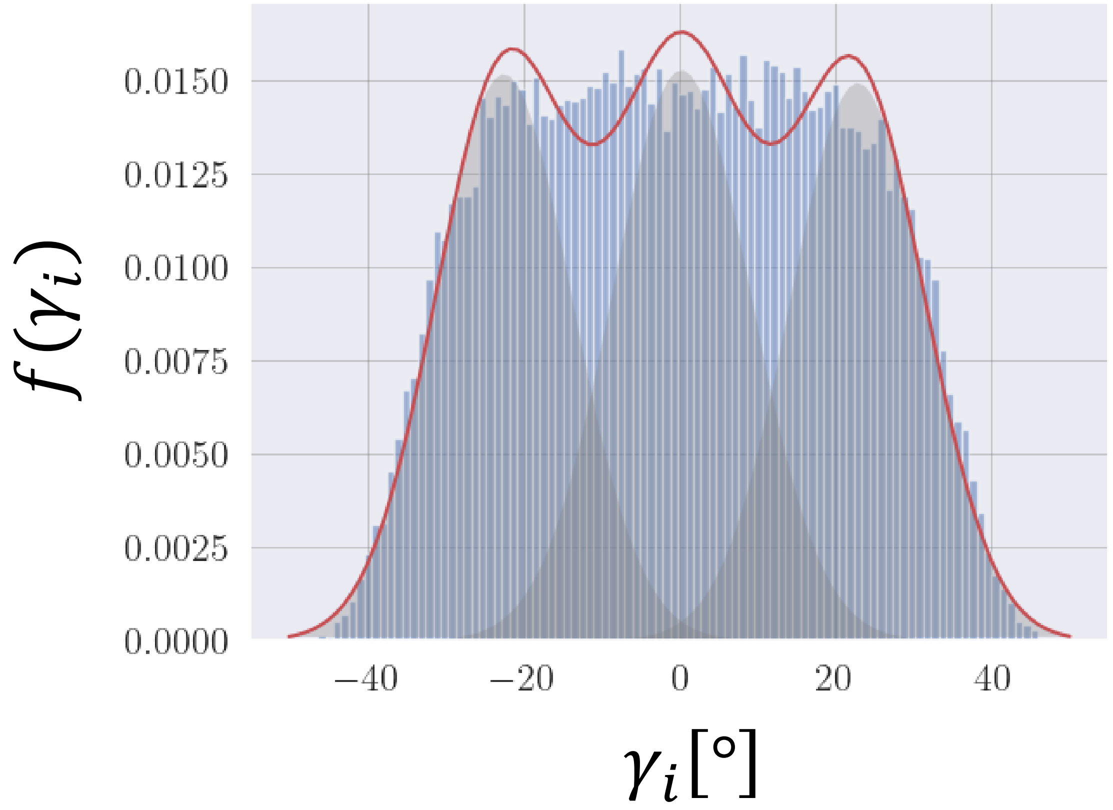


Deconvolution of Super-Gaussian Distributions





Bayesian Inference – Results



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

Likelihood Function

$$rob(\dot{m}(\theta)_{UCLA}|\gamma_i,I) = \prod_i^N \sum_{j=1}^{k} \alpha_j prob(\dot{m}(\theta)_i|\gamma_i,I)$$

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

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

Prior Distributions

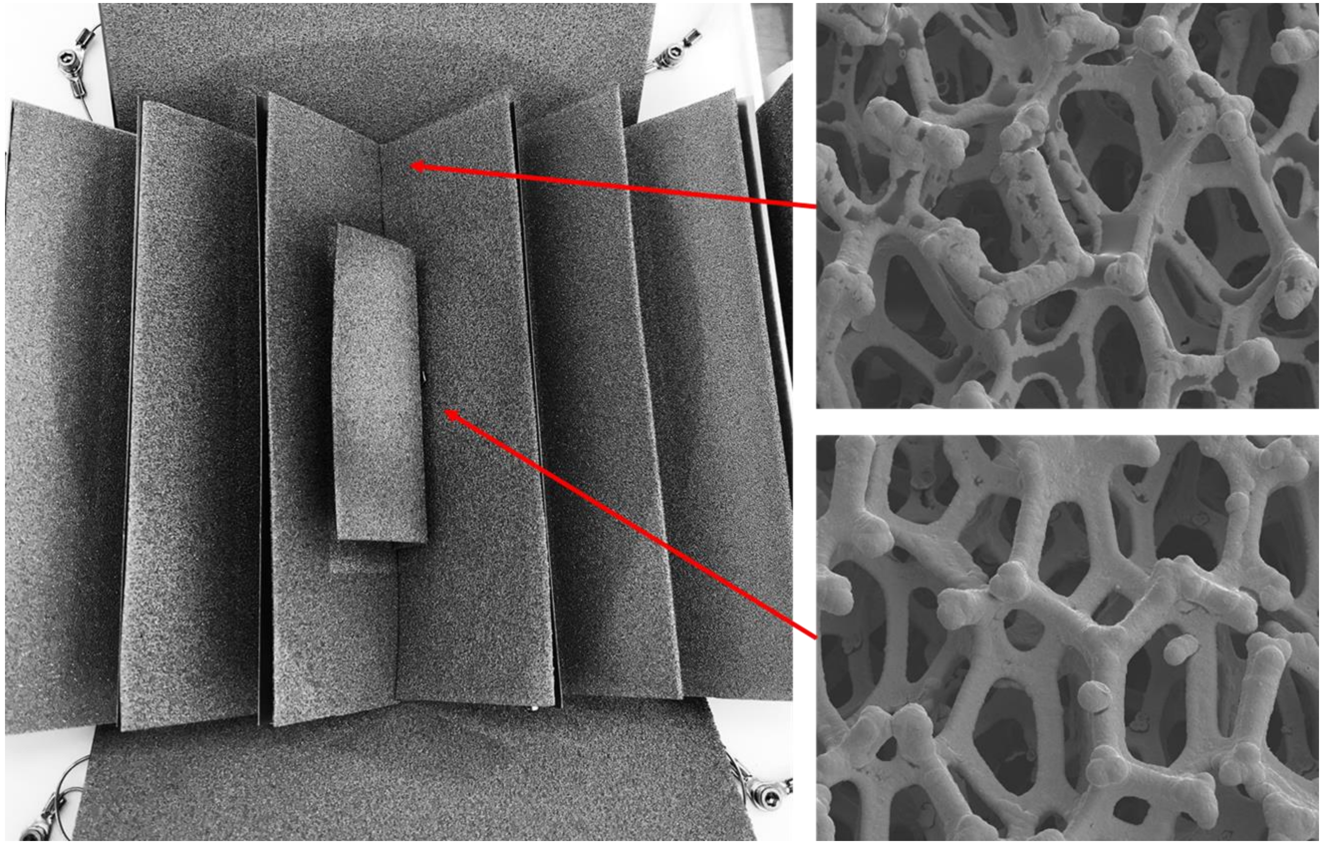
$A_1 \sim \mathcal{N}(200, 100)$; $\mu_1 \sim \mathcal{N}(0, 10^{-3})$;

$\sigma_1 \sim \mathcal{N}(100, 50)$; $n_1 \sim \mathcal{N}(1.5, 1)$

$\mathbf{k = 3; \alpha \sim \{1.0, 0.0, 0.0\}}$

Super-Gaussian-based profiles data generating process results in Gaussian behavior of multiple “sources” of emission.

Gaussian Mixture Modeling



- Threshold analysis shows onset of shock-induced desorption when primary droplets from electrospray plume strike beam target [1]
- Deconvolved results may provide insight into why certain population desorb or stay below the desorption threshold

[1] Uchizono, N. M., Wright, P. L., Collins, A. L., Chamieh, M. C., Chandrasekar, K., and Wirz, R. E., "Electrospray Thruster Facility Effects: Characterization and Mitigation," International Electric Propulsion Conference, ERPS, 2022, p. 219.

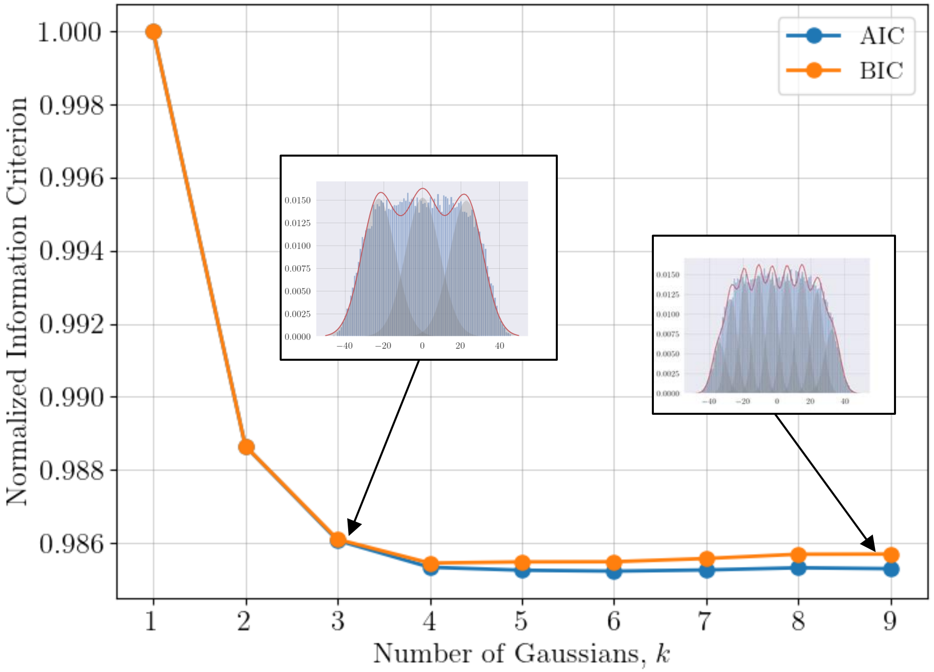
- Optimal number of Gaussian components determined by…
  - *Aikaki Information Criterion (AIC)*

    $$\boldsymbol{AIC = -2\log(\hat{L}) + 2d}$$

  - *Bayesian Information Criterion (BIC)*

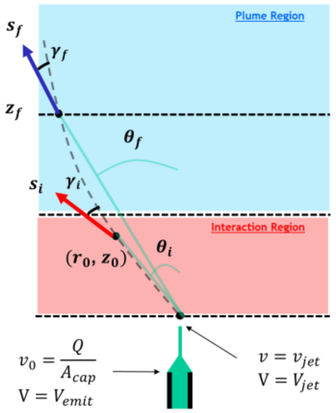
    $$\boldsymbol{BIC = -2\log(\hat{L}) + \log(N)\, d}$$

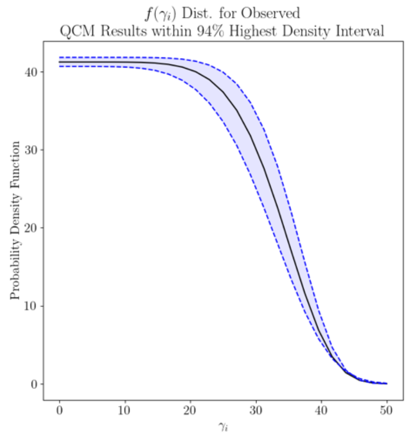
  where $\hat{L}$ is the maximum likelihood of the model, d is the number of parameters ($d \propto k$), and N is the number of samples

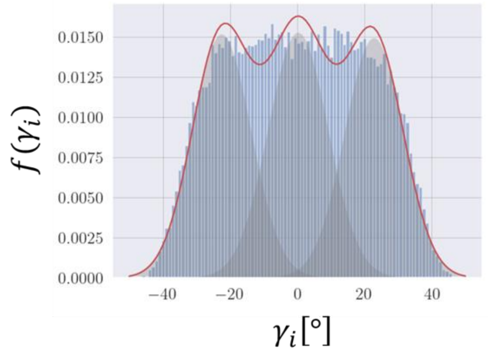


Conclusions

- A data-driven computational framework has been developed to investigate super-Gaussian mass flux profiles observed in QCM experiments
- Results based on provided data sets suggest most probable functional form of $\boldsymbol{\gamma_i}$ must also follow Super-Gaussian shape.
- Super-Gaussian-based profiles data generating process results in Gaussian behavior of multiple "sources" of emission.
- Future work includes…
  - Mass to current density mapping
  - Identifying species information from GMM results
  - Providing plume profiles in varied electrospray domains



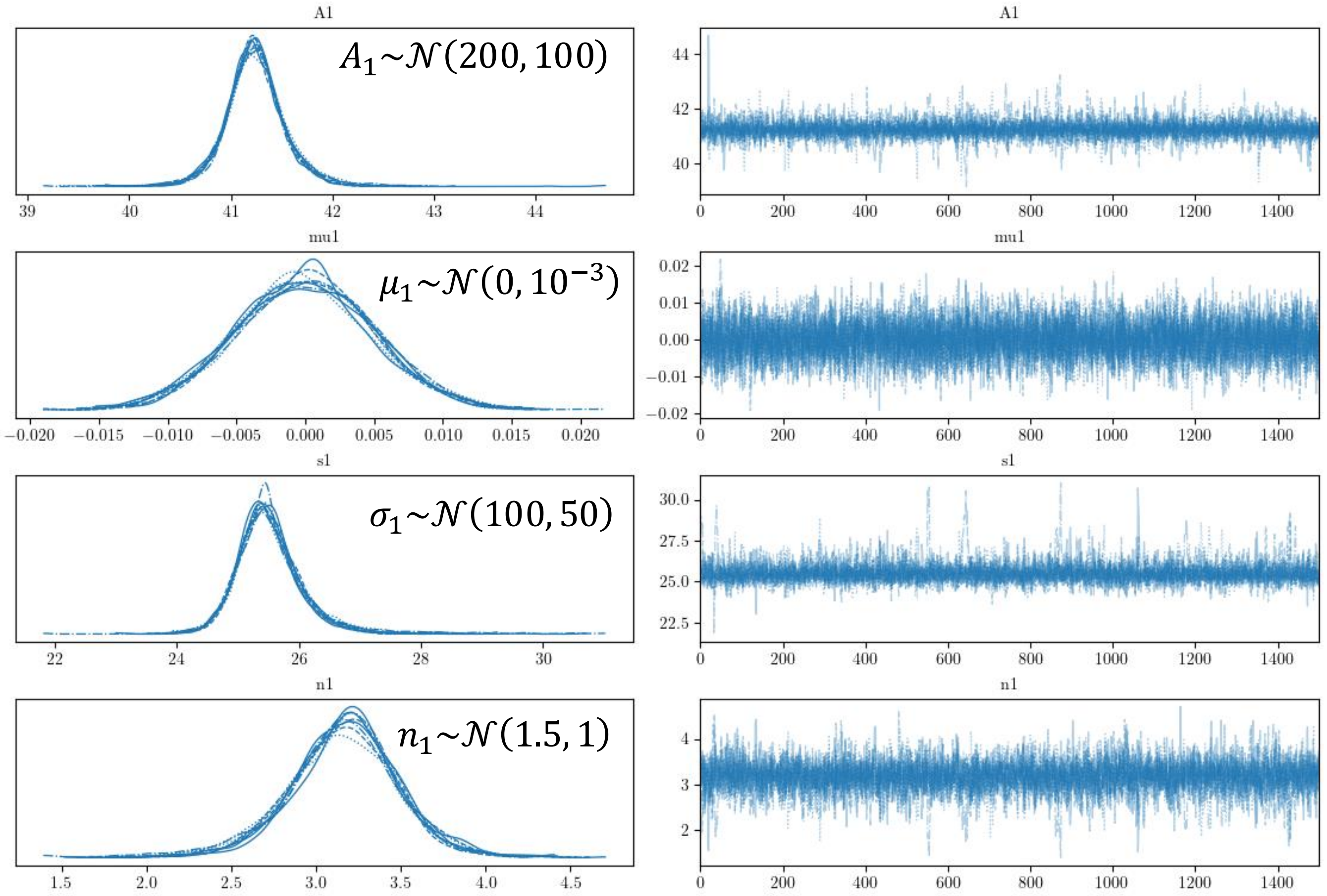




Shehan Parmar, shehan.parmar@gmail.com
Richard E. Wirz, wirz@ucla.edu

Thank You! Questions?

BONUS: Parameter Posteriors



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

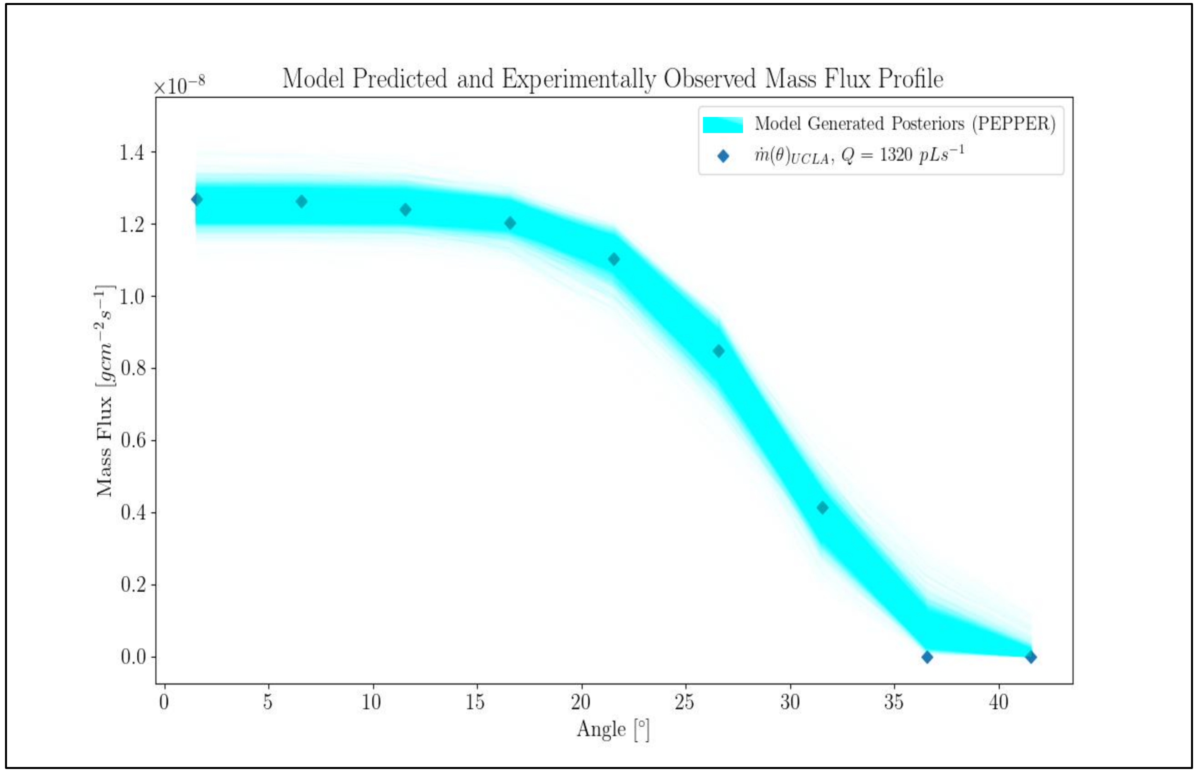
$$prob(\dot{m}(\theta)_{UCLA}|\gamma_i, I) = \prod_i^N prob(\dot{m}(\theta)_i|\gamma_i, I)$$

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

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

BONUS: 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.

BONUS: What is a Sobol Index?

<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 $\mathbb{M}_{PCE}$: $\boldsymbol{\theta_i}, \boldsymbol{\gamma_i}, \mathbf{V_{acc}} \rightarrow \theta_f$?

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

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

Suppose we have a function, $f(\boldsymbol{X})$, where $\mathrm{X} = \mathrm{X}_1, \mathrm{X}_2, \ldots, X_i$ 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]:

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

*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 $V_u (u \in [1, \ldots, p])$ is the *interactive variance* contribution of X_u (one can think of it as a conditional variance, where $V_u = V(f(X_i)|X_i)$):

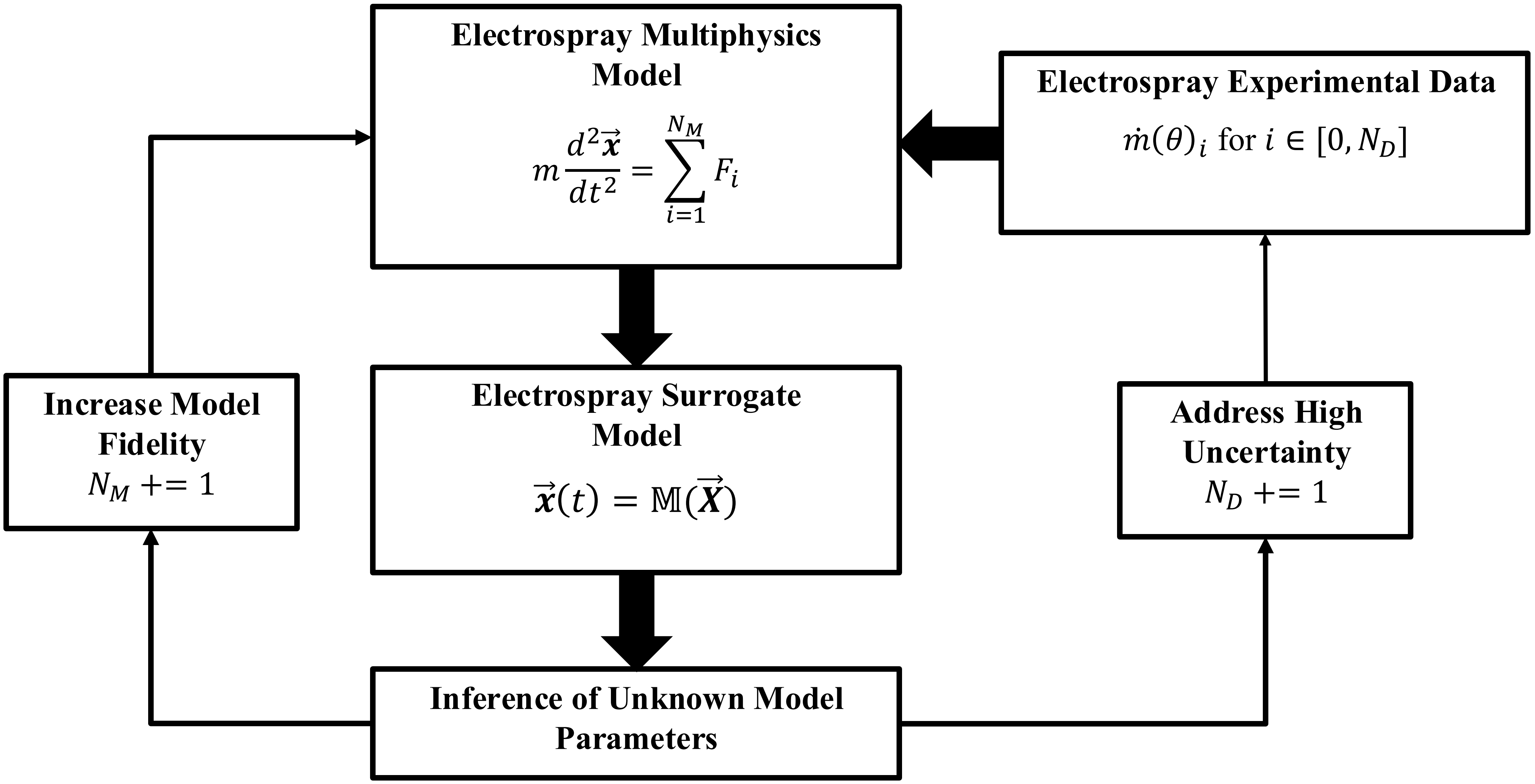
$$V = \sum_{i=1}^{p} V_i + \sum_{1 \le i \le j \le p} V_{ij} + \cdots + V_{1,2,\ldots,p}$$

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>.

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

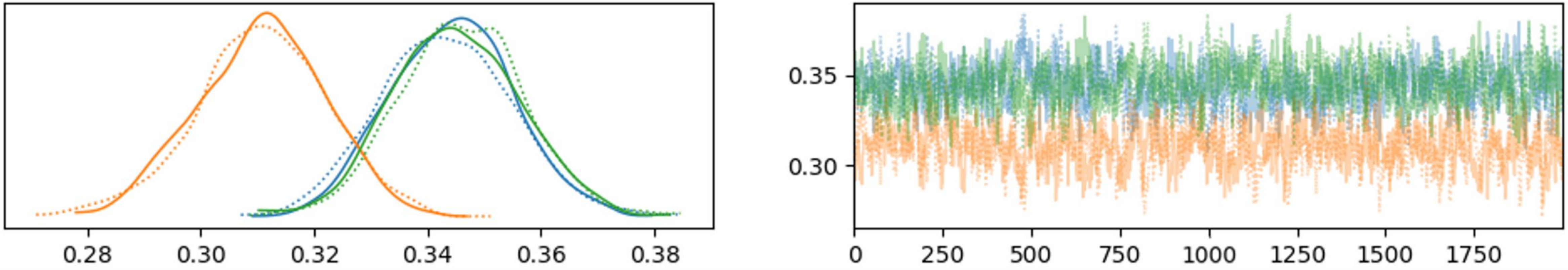
[1] Sobol IM (1993) Sensitivity estimates for nonlinear mathematical models. Math model comput exp 1(1):112–118
[2] Sudret B (2008) Global sensitivity analysis using polynomial chaos expansions. Reliab Eng Syst Saf 93(7):964–979

BONUS: Iterative Plume Modeling Paradigm

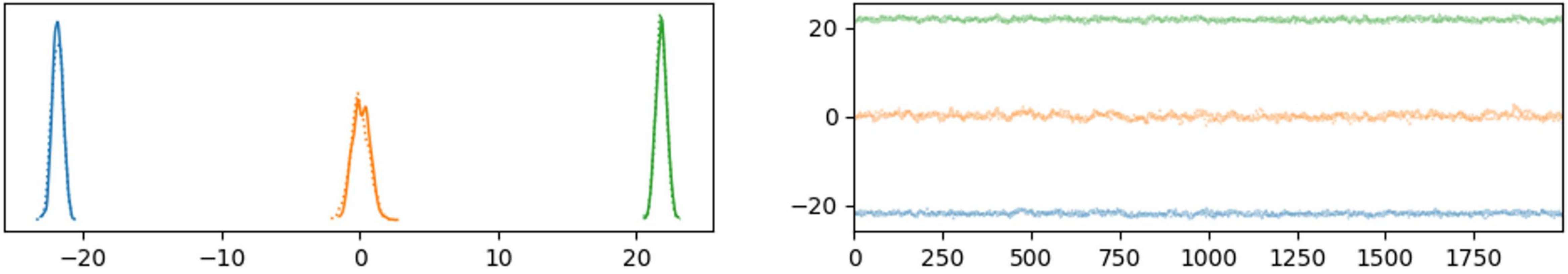


BONUS: Mixture Modeling Trace Plots

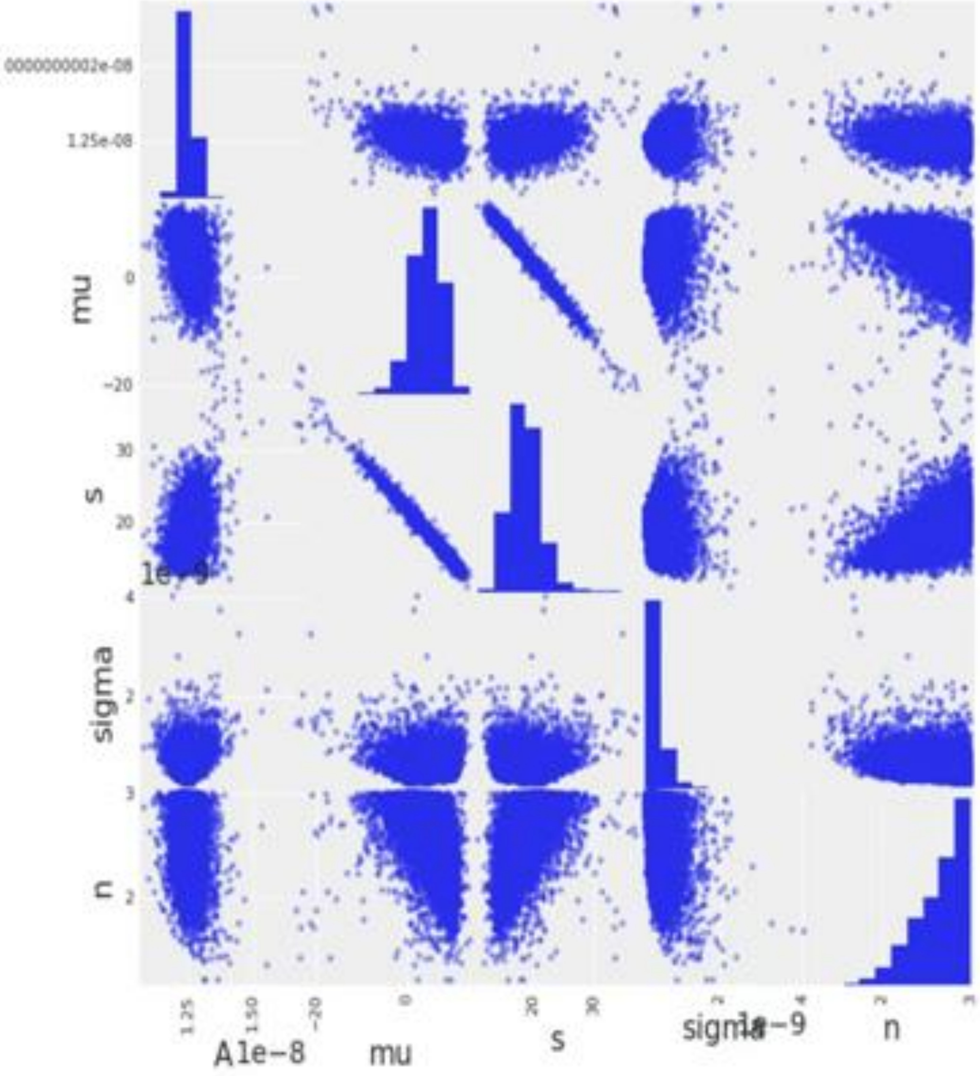
$f(\alpha_i)$



$f(\gamma_{\mu_i})$



BONUS: Noise Model Corner Plot



Plume Scale

Plume Tilt

<u>**Gaussian Noise**</u>

Plume Width/Std. Deviation

Plume Sharpness