APPENDIX C

WHEN PHYSICS-INFORMED DATA ANALYTICS OUTPERFORMS BLACK-BOX MACHINE LEARNING: A CASE STUDY IN THICKNESS CONTROL FOR ADDITIVE MANUFACTURING

TABLE C.1

THIS TABLE REPORTS THE TRANSFORMATIONS (I.E., RESCALING COEFFICIENTS) FOR EACH DECISION VARIABLE AND MEASUREMENT.

variable	Voltage (V)	Speed ($mm \cdot s^{-1}$)	Carrier gas flowrate ($cm^3 \cdot min^{-1}$)	Sheath flow ($cm^3 \cdot min^{-1}$)	Thickness (μm)
γ	50	1	25	90	1

TABLE C.2

THIS TABLE REPORTS THE RESULTS FROM REGRESSING THE 1D MODELS g_1, g_2, AND g_3.

Runs	Model	Estimated Parameters
2, 5, 6, 7, 8, 9, 10	$g_1(U) = \frac{1}{1+\exp\{-\alpha_1 U + \alpha_0\}}$	$\alpha_1 = 30.99, \alpha_0 = 15.38$
5, 11, 12, 13	$g_2(Q_a, Q_s^*) = aQ_a + b$	$a = 0.11, b = -1.03$
19, 20, 21, 22	$g_2(Q_a, Q_s^*) = aQ_a + b$	$a = 0.13, b = -1.32$
5, 14, 15, 16, 17, 18, 20	$g_2(Q_a^*, Q_s) = aQ_s^2 + Q_s b + c$	$a = -3.35^{-4}, b = 3.48 \times 10^{-2}$, $c = -4.05$
1, 2, 3, 4	$g_3(v_p) = \frac{1}{v_p}$	

TABLE C.3

THIS TABLE SUMMARIZES THE REGRESSED PARAMETERS FOR MODELS IN THE LIBRARY.

	model 0	model 1	model 2	model 3	model 4	model 5	model 6	model 7
β_{00}	-0.1219	-0.0113	0.0005	-0.0092	-0.0140	-0.0087	-0.0085	0.0014
β_{10}	0.3162	0.0281	-0.0033	0.0229	0.0184	0.0277	0.0102	-0.0050
β_{20}	-0.2025	-0.0204	0	-0.0174	0	-0.0255	0	0
β_{01}	0.2116	0.0154	0.0051	0.0115	0.0307	0.0089	0.0160	0.0085
β_{11}	-0.5171	-0.0097	0.0441	0	-0.0325	0	0	0
β_{21}	0.3186	0	-0.0343	-0.0058	0	0	-0.0157	0
$\hat{\sigma}^2$	0.0150	0.0171	0.0177	0.0172	0.0251	0.0172	0.0195	0.0484

TABLE C.4

THIS TABLE REPORTS THE EIGENDECOMPOSITION AND CONDITION NUMBER OF THE FISHER INFORMATION MATRIX AND ASSOCIATED IDENTIFIABILITY.

2*Model	2*Eigenvalues	Eigenvectors						2*Condition Number	2*Identifiable
		β_{00}	β_{10}	β_{20}	β_{01}	β_{11}	β_{21}		
6*0	1.69E+09	2.90E-01	-5.82E-01	3.00E-01	-2.82E-01	5.67E-01	-2.93E-01	6*1.82E+16	6*No
	2.67E+07	5.31E-01	9.49E-03	-4.67E-01	-5.21E-01	-2.72E-02	4.77E-01		
	4.25E+06	-2.31E-01	6.02E-01	-2.69E-01	-3.15E-01	5.50E-01	-3.32E-01		
	9.73E+05	-3.88E-01	-3.64E-01	-4.63E-01	3.59E-01	4.58E-01	4.05E-01		
	9.69E+03	5.10E-01	-1.27E-02	-4.88E-01	5.02E-01	-2.38E-02	-4.98E-01		
	9.30E-08	4.11E-01	4.08E-01	4.08E-01	4.10E-01	4.06E-01	4.05E-01		
5*1	9.53E+04	6.09E-01	-5.75E-01	2.98E-01	-4.58E-01	2.38E-02		5*2.23E+7	5*Yes
	2.04E+03	4.60E-01	4.73E-01	-6.37E-01	-3.98E-01	-1.78E-02			
	1.22E+02	-5.16E-01	2.19E-01	2.75E-01	-7.79E-01	5.61E-02			
	3.28E+01	-3.87E-01	-6.29E-01	-6.55E-01	-1.48E-01	5.35E-02			
	4.27E-03	4.35E-02	4.36E-02	1.19E-03	5.56E-02	**9.97E-01**			
5*2	4.84E+04	4.18E-01	2.21E-02		-2.27E-01	-7.74E-01	4.17E-01	5*2.77E+7	5*Yes
	9.57E+02	-6.77E-01	-1.96E-04		3.40E-01	-1.20E-01	6.41E-01		
	4.29E+01	-5.48E-01	-3.25E-02		-1.74E-01	-5.65E-01	-5.92E-01		
	1.21E+01	-2.52E-01	-1.09E-01		-8.91E-01	2.58E-01	2.54E-01		
	1.74E-03	5.50E-02	**-9.93E-01**		9.81E-02	-2.70E-02	6.67E-04		
5*3	8.95E+04	6.15E-01	-5.68E-01	2.95E-01	-4.60E-01		1.24E-02	5*2.01E+7	5*Yes
	1.90E+03	4.55E-01	4.80E-01	-6.39E-01	-3.93E-01		-2.64E-02		
	1.16E+02	-5.19E-01	2.13E-01	2.69E-01	-7.82E-01		4.65E-02		
	3.03E+01	-3.80E-01	-6.34E-01	-6.57E-01	-1.47E-01		-1.39E-02		
	4.28E-03	2.32E-02	9.70E-04	-4.22E-02	2.97E-02		**9.98E-01**		
4*4	8.42E+03	2.77E-01	-6.72E-01		-1.25E-01	6.75E-01		4*1.13E+6	4*Yes
	4.12E+01	-8.66E-01	-8.17E-02		3.56E-01	3.40E-01			
	1.96E+01	6.94E-02	7.18E-01		-2.74E-01	6.36E-01			
	7.44E-03	4.09E-01	1.60E-01		**8.85E-01**	1.55E-01			
4*5	9.25E+04	6.08E-01	-5.74E-01	3.12E-01	-4.52E-01			4*2.81E+3	4*Yes
	2.04E+03	-4.66E-01	-4.52E-01	6.49E-01	3.96E-01				
	1.17E+02	5.03E-01	-2.35E-01	-2.80E-01	7.83E-01				
	3.28E+01	-4.00E-01	**-6.41E-01**	**-6.35E-01**	-1.62E-01				
4*6	1.56E+05	6.84E-01	-4.07E-01		-5.67E-01		2.12E-01	4*6.58E+3	4*Yes
	2.26E+03	-3.21E-01	-5.98E-01		2.94E-01		6.73E-01		
	3.54E+02	4.87E-01	-3.55E-01		6.97E-01		-3.88E-01		
	2.37E+01	4.38E-01	**5.93E-01**		3.25E-01		**5.93E-01**		

TABLE C.5

THIS TABLE COMPARES THE ESTIMATED PARAMETERS OBTAINED VIA TRAINING USING THE ORIGINAL DATA WITH AND WITHOUT THE AUGMENTED DATA FOR ALL MODELS.

	model 0		model 1		model 2		model 3		model 4		model 5		model 6		model 7	
parameter	before	after	before	after	before	after	before	after	before	after	before	after	before	after	before	after
β_{00}	-1.1242	0.0148	-0.0189	-0.0374	-0.0094	-0.0223	-0.0185	-0.026	0.0057	-0.0327	-0.018	-0.0116	-0.028	-0.0268	-0.0093	0.0023
β_{10}	3.678	-0.0809	0.0303	0.0607	-0.0008	0.0199	0.029	0.0297	-0.0231	0.0391	0.029	0.0336	0.0287	0.0261	0.0008	-0.0019
β_{20}	-3.0099	0.0655	-0.0255	-0.0264	0	0	-0.0244	-0.0061	0	0	-0.0255	-0.0314	0	0	0	0
β_{01}	2.0001	-0.0339	0.0262	0.059	0.0094	0.0321	0.0255	0.0388	-0.0048	0.0644	0.0248	0.0116	0.0428	0.0418	0.0222	0.0034
β_{11}	-6.5159	0.1963	-0.0023	-0.0551	0.0533	0.0177	0	0	0.0428	-0.069	0	0	0	0	0	0
β_{21}	5.3293	-0.1625	0	0	-0.0455	-0.047	-0.0019	-0.0359	0	0	0	0	-0.0453	-0.0407	0	0

TABLE C.6

THIS TABLE SUMMARIZES THE LEAVE-ONE-OUT MEAN SQUARED ERROR (LOO-MSE) FOR MODELS 0, 1, 3, 5, AND GPR.

Model	model 5	GPR	model 0	model 3	model 5
LOO-MSE	0.024	0.020	326.92	0.69	1.20

TABLE C.7

THIS TABLE COMPARES THE PARAMETER UNCERTAINTY (DIAGONAL OF THE COVARIANCE MATRIX) WHEN MODEL 5 IS TRAINED WITH ORIGINAL DATA (RUNS 1 TO 22) AND WITH THE AUGMENTED DATA (RUNS 1 TO 23).

Parameters Standard Deviation	β_{00} $(\mathrm{cm}^3 \cdot \mathrm{min}^{-1})$	β_{10} dimensionless	β_{20} $(\mathrm{min} \cdot \mathrm{cm}^{-3})$	β_{01} dimensionless
Original (runs 1 to 22)	0.0015	0.00331	0.00292	0.00193
Augmented (runs 1 to 23)	0.0027	0.0068	0.0058	0.0021

TABLE C.8

THIS TABLE REPORTS THE LEAVE-ONE-OUT MEAN SQUARED ERROR (LOO-MSE) OF MODEL 5 AND GPR IN HIGH- AND LOW-THICKNESS REGIONS.

	model 5	GPR
high thickness $h \geq 0.9\mu$m	0.0576	0.0832
low thickness $h < 0.9\mu$m	0.0157	0.0051

Algorithm 2 Calculate the difference between estimated parameters and sampled parameters in A-, D- and E-optimality

Given: Estimated parameters $\hat{\boldsymbol{\beta}}$, estimated uncertainty $\hat{\sigma}$, dataset $\mathbb{D}$, variance-covariance matrix of estimated parameters $\hat{\Sigma}_{\hat{\boldsymbol{\beta}}}$, new experiments $\mathbf{X}_*$
Sample $\tilde{\mathbf{z}}$, where $\mathbf{z} \sim N(\mathbf{0}, \mathbf{I}_p)$
Calculate $\tilde{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}} + \hat{\Sigma}_{\hat{\boldsymbol{\beta}}}^{\frac{1}{2}} \cdot \tilde{\mathbf{z}}$, where $\tilde{\boldsymbol{\beta}} \sim N(\hat{\boldsymbol{\beta}}, \hat{\Sigma}_{\hat{\boldsymbol{\beta}}})$
Calculate $\hat{\mathbf{M}} = \sum\limits_{i \in \mathbb{D}} \mathbf{M}_i = \mathbf{M}(\hat{\boldsymbol{\beta}}, \mathbf{x}_i, \hat{\sigma})$, $\tilde{\mathbf{M}} = \sum\limits_{i \in \mathbb{D}} \mathbf{M}_i = \mathbf{M}(\tilde{\boldsymbol{\beta}}, \mathbf{x}_i, \hat{\sigma})$
for $\mathbf{x}_j$ in $\mathbf{X}_*$ **do**
    Calculate $\hat{\mathbf{M}}_j = \hat{\mathbf{M}} + \mathbf{M}(\hat{\boldsymbol{\beta}}, \mathbf{x}_j, \hat{\sigma})$, $\tilde{\mathbf{M}}_j = \tilde{\mathbf{M}} + \mathbf{M}(\tilde{\boldsymbol{\beta}}, \mathbf{x}_j, \hat{\sigma})$
    Eigendecomposition $\hat{\lambda_j^k}, \tilde{\lambda_j^k}$, where $k \in \{1, 2, \cdots, p\}$
    Calculate $A_j = \sum\limits_{k=1}^{p} \hat{\lambda_j^k} - \sum\limits_{k=1}^{p} \tilde{\lambda_j^k}$, $D_j = \prod_{k=1}^{p} \hat{\lambda_j^k} - \prod_{k=1}^{p} \tilde{\lambda_j^k}$, $E_j = \min\{\hat{\lambda_j^k}\} - \min\{\tilde{\lambda_j^k}\}$
end for
Return: $\mathbf{A}, \mathbf{D}, \mathbf{E}$

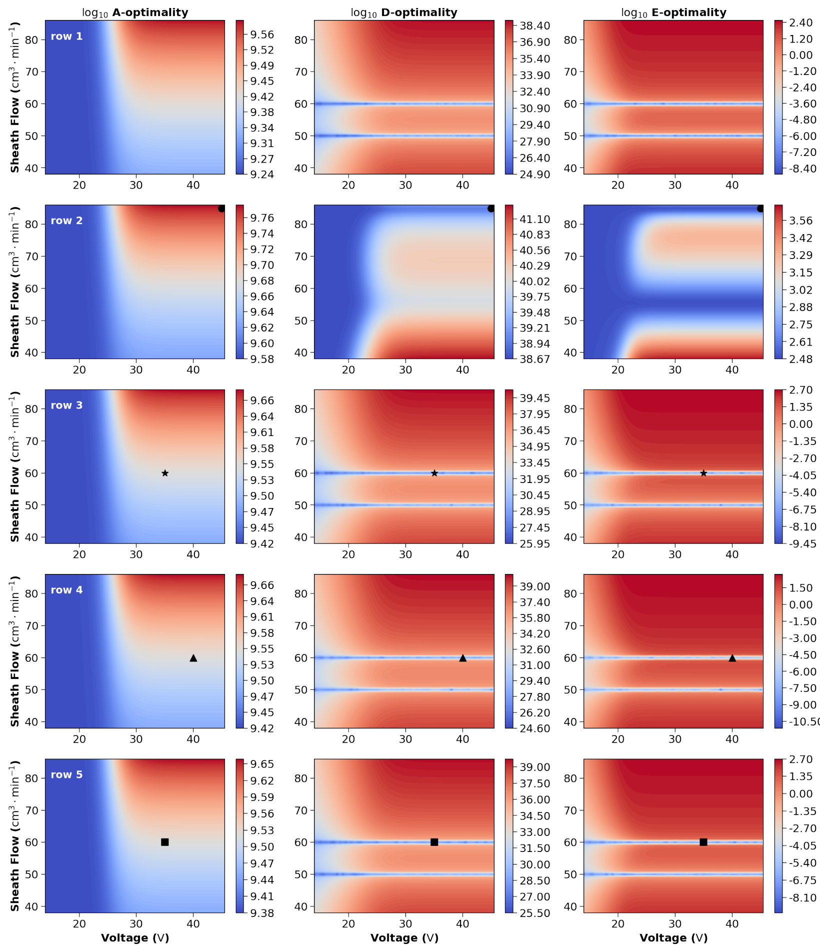

Figure C.1. This figure shows the sensitivity of A-, D-, and E-optimality metrics for model 0 when a new experiment is added. Detailed description is given in Figure 5.5. As discussed in the main text, model 0 is not identifiable with the original data. For illustration purposes, we compute the absolute value of Eqs. (5.23) and (5.24). The two horizontal lines at $Q_s = 50\ \mathrm{cm}^3 \cdot \mathrm{min}^{-1}$ and $Q_s = 60\ \mathrm{cm}^3 \cdot \mathrm{min}^{-1}$ are because the dataset already contains information at these experimental conditions, so adding another experiment does not improve the identifiability (smallest eigenvalue). Except for the two horizontal lines, the model is identifiable after adding other new experiments. The result indicates the unidentifiable of model 0 is caused by a practical identifiability problem with not enough experimental data.

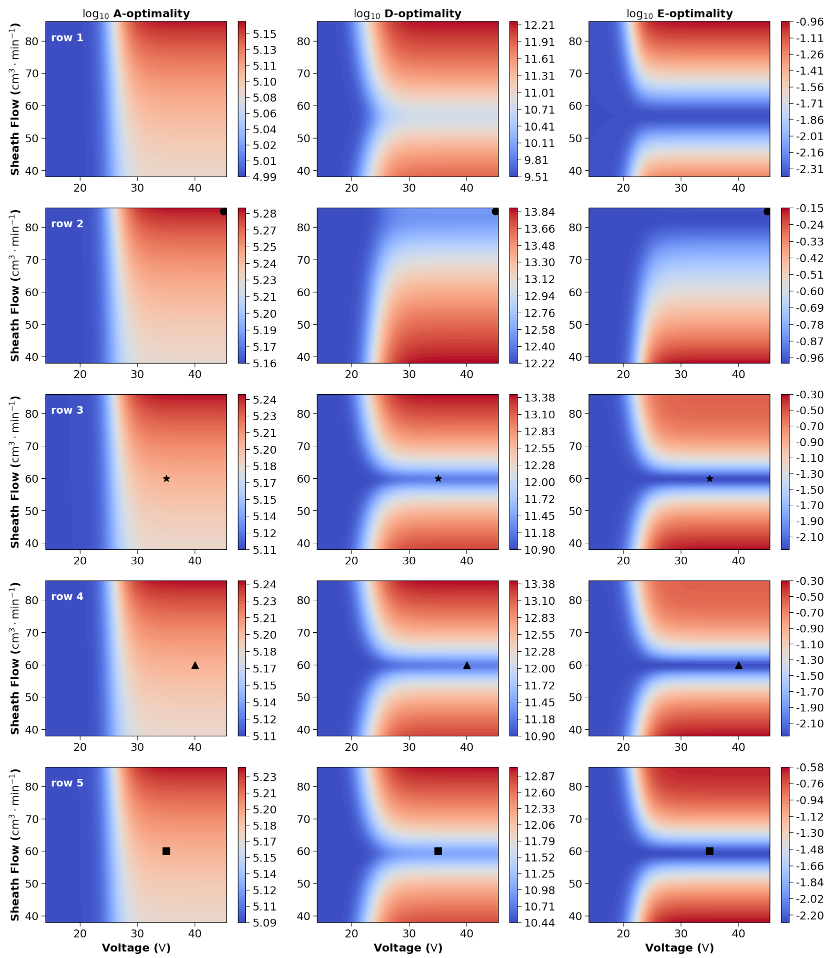

Figure C.2. This figure shows the sensitivity of A-, D-, and E-optimality metrics for model 1 when a new experiment is added. Detailed description is given in Figure 5.5.

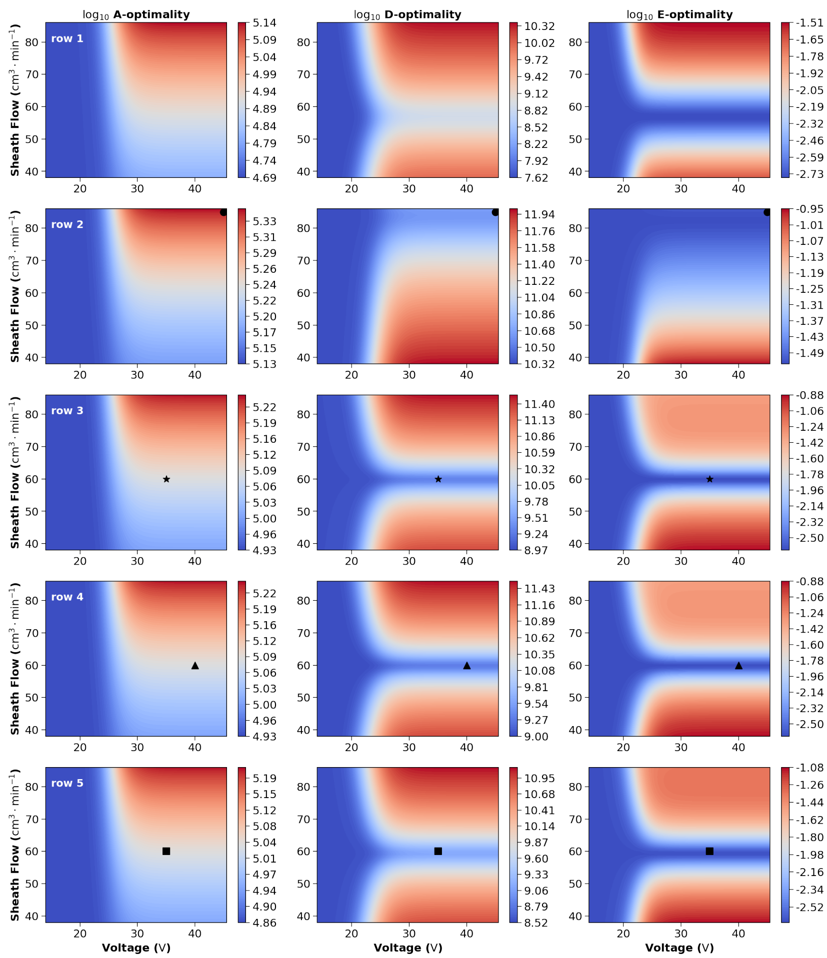

Figure C.3. This figure shows the sensitivity of A-, D-, and E-optimality metrics for model 2 when a new experiment is added. Detailed description is given in Figure 5.5.

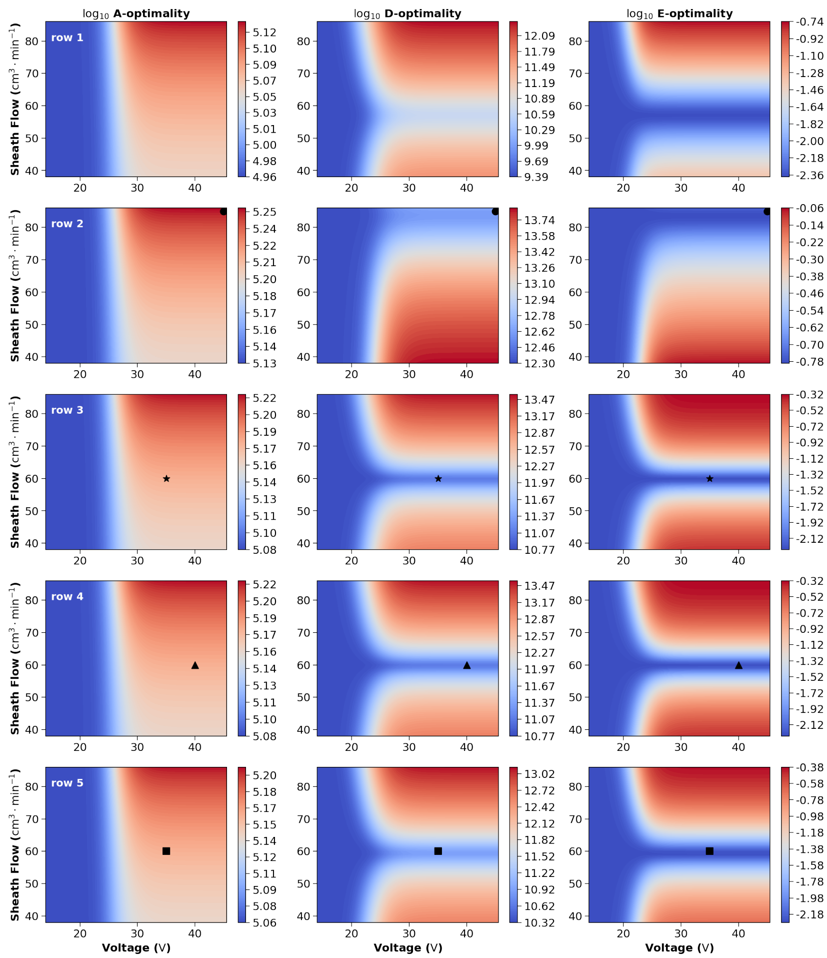

Figure C.4. This figure shows the sensitivity of A-, D-, and E-optimality metrics for model 3 when a new experiment is added. A detailed description is given in Figure 5.5.

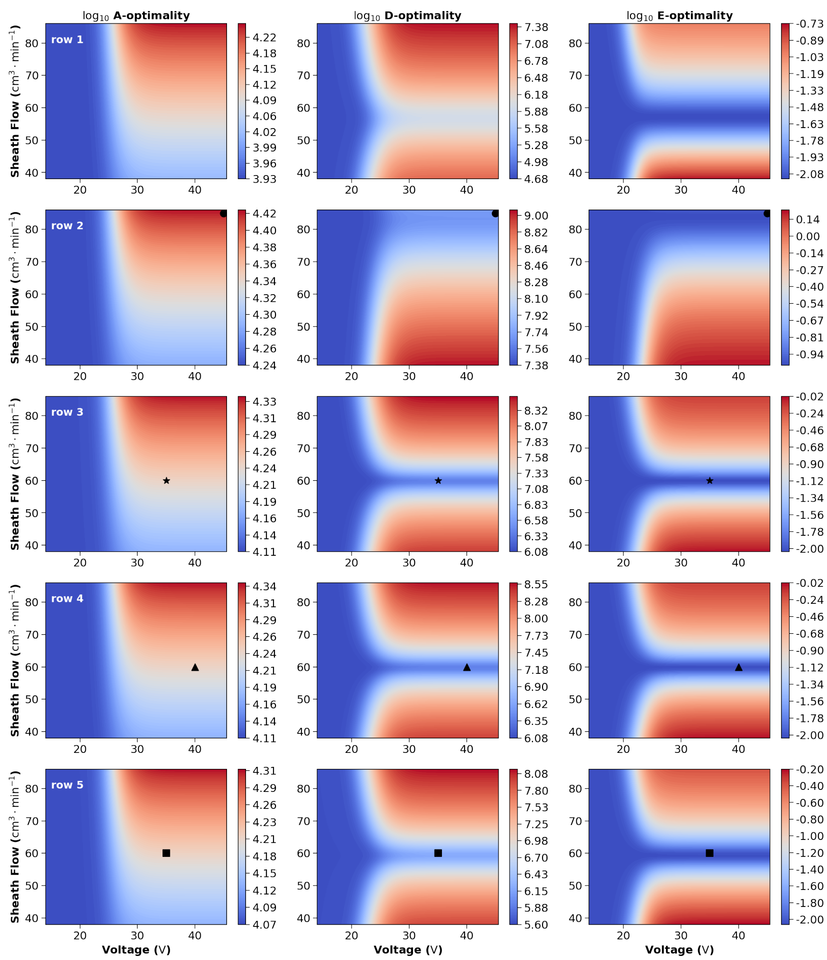

Figure C.5. This figure shows the sensitivity of A-, D-, and E-optimality metrics for model 4 when a new experiment is added. Detailed description is given in Figure 5.5.

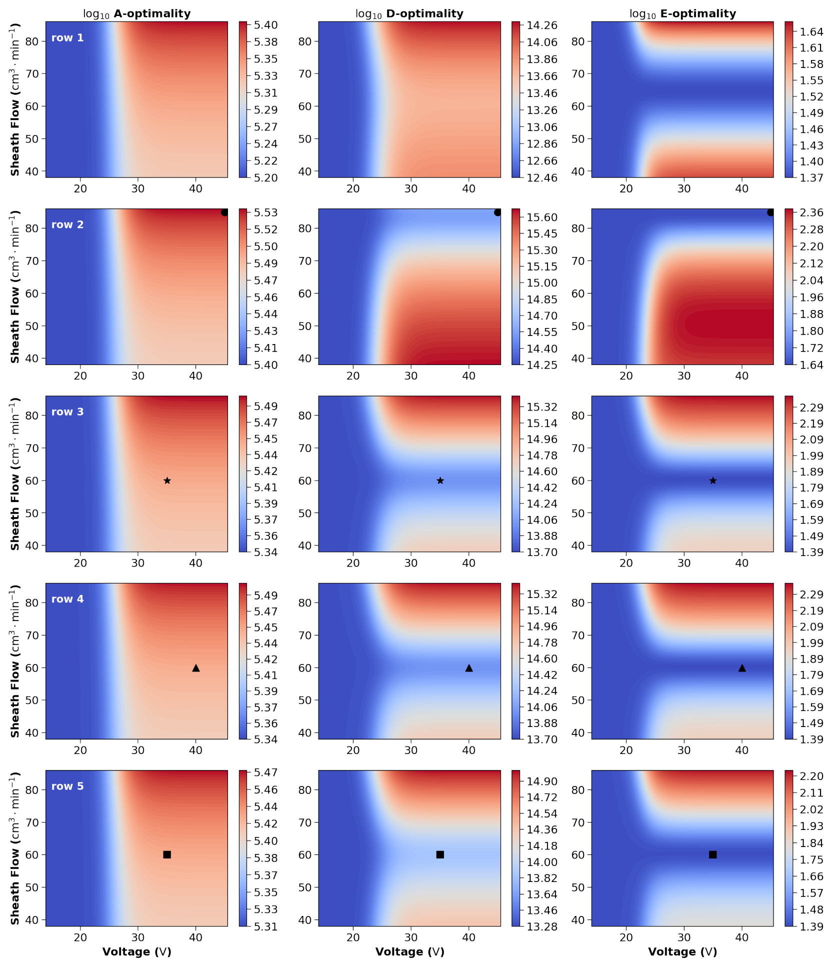

Figure C.6. This figure shows the sensitivity of A-, D-, and E-optimality metrics for model 6 when a new experiment is added. Detailed description is given in Figure 5.5.

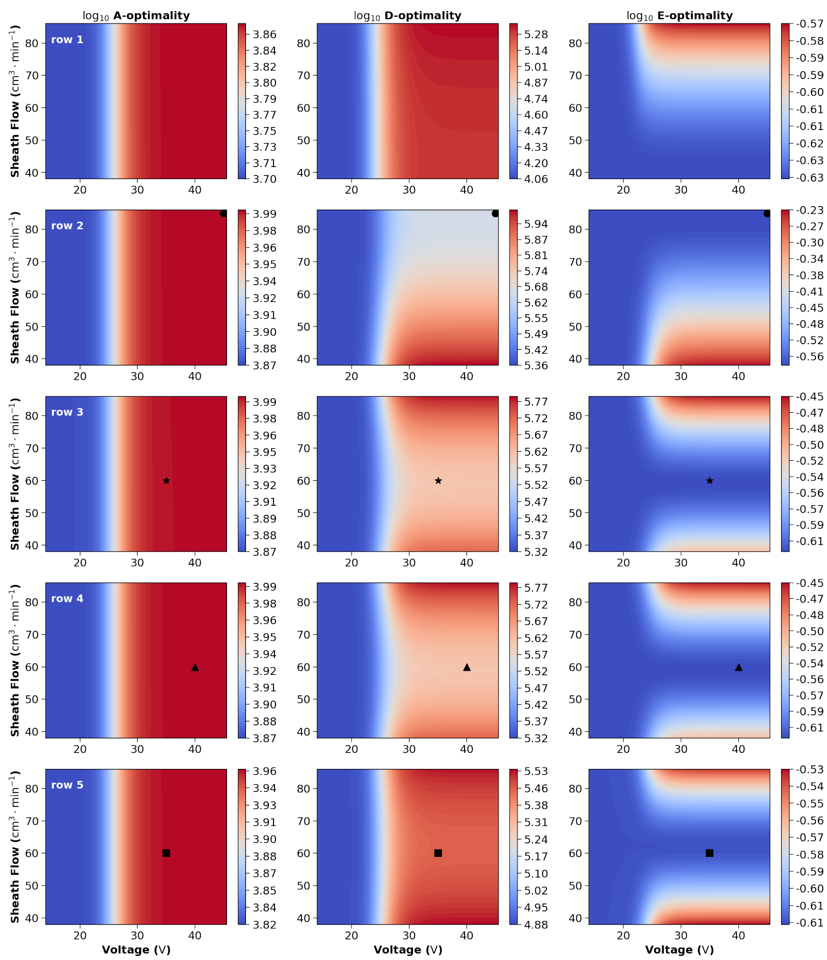

Figure C.7. This figure shows the sensitivity of A-, D-, and E-optimality metrics for model 7 when a new experiment is added. Detailed description is given in Figure 5.5.

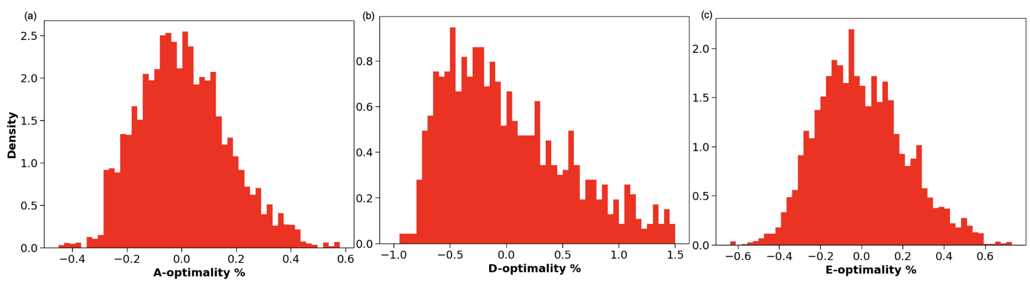

Figure C.8. This figure shows the histogram of the percent differences in A-, D-, and E-optimality metrics between sampled parameters and optimal parameters. From this figure, we conclude the MBDoE metrics as insensitivity to parameter uncertainty.

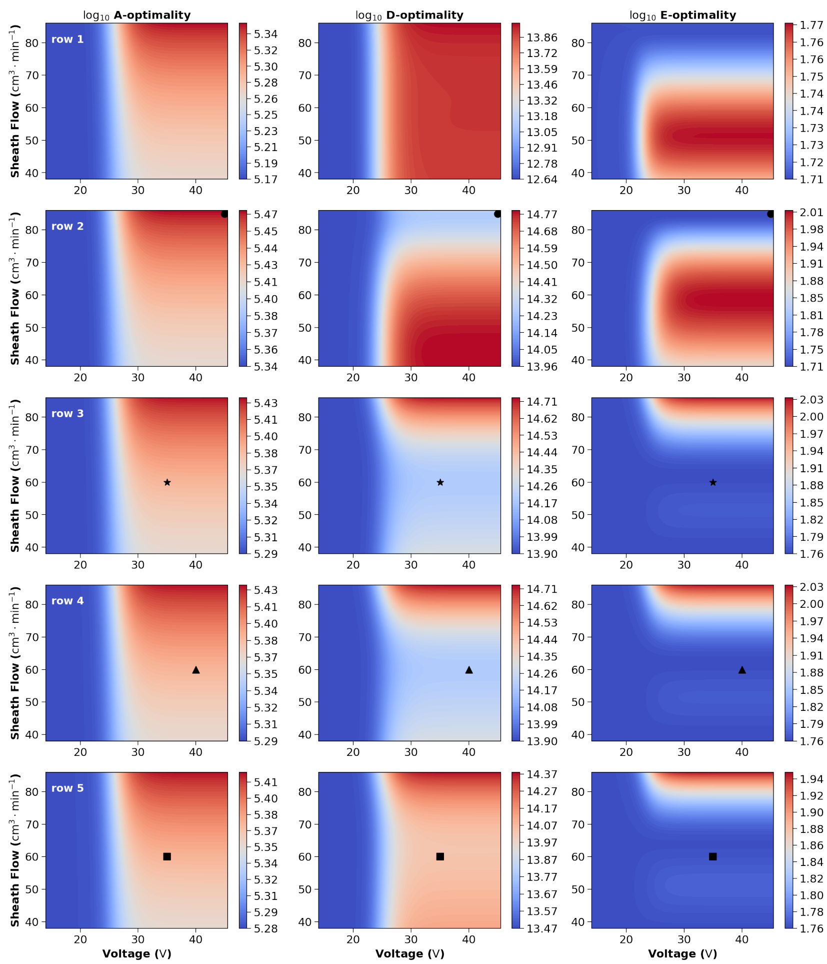

Figure C.9. This figure shows the sensitivity of A-, D-, and E-optimality metrics, computed with model parameters $\beta_{00} = -0.023, \beta_{10} = 0.036, \beta_{20} = -0.032, \beta_{01} = 0.031$, in model 5 when a new experiment is added.

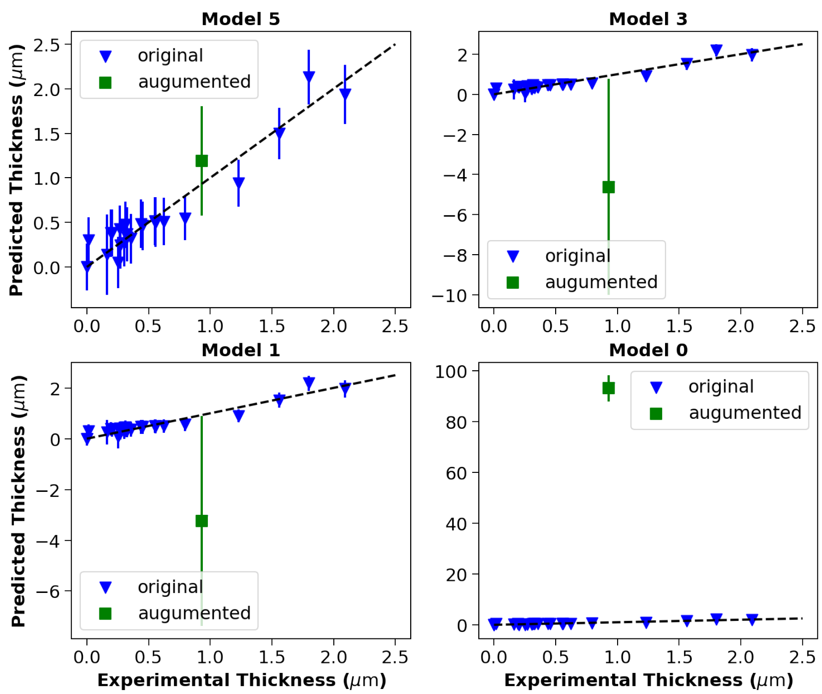

Figure C.10. This parity plot shows the leave-one-out prediction of the models 0, 1, 3, and 5. The error bars are the 95% PI calculated via Eq. (5.16).

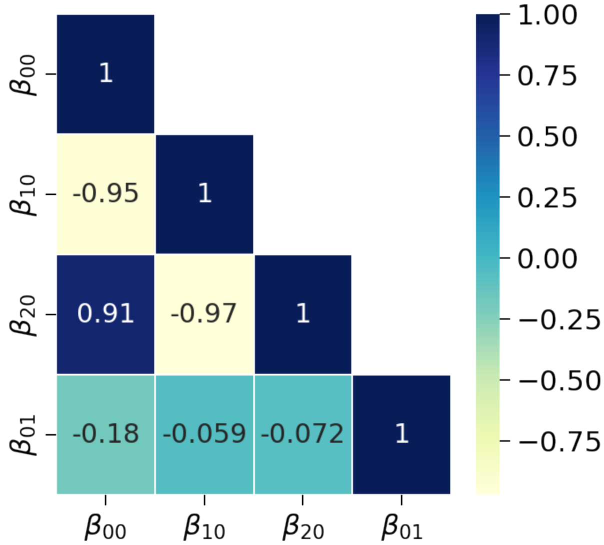

Figure C.11. This figure shows the correlation between parameters for model 5.

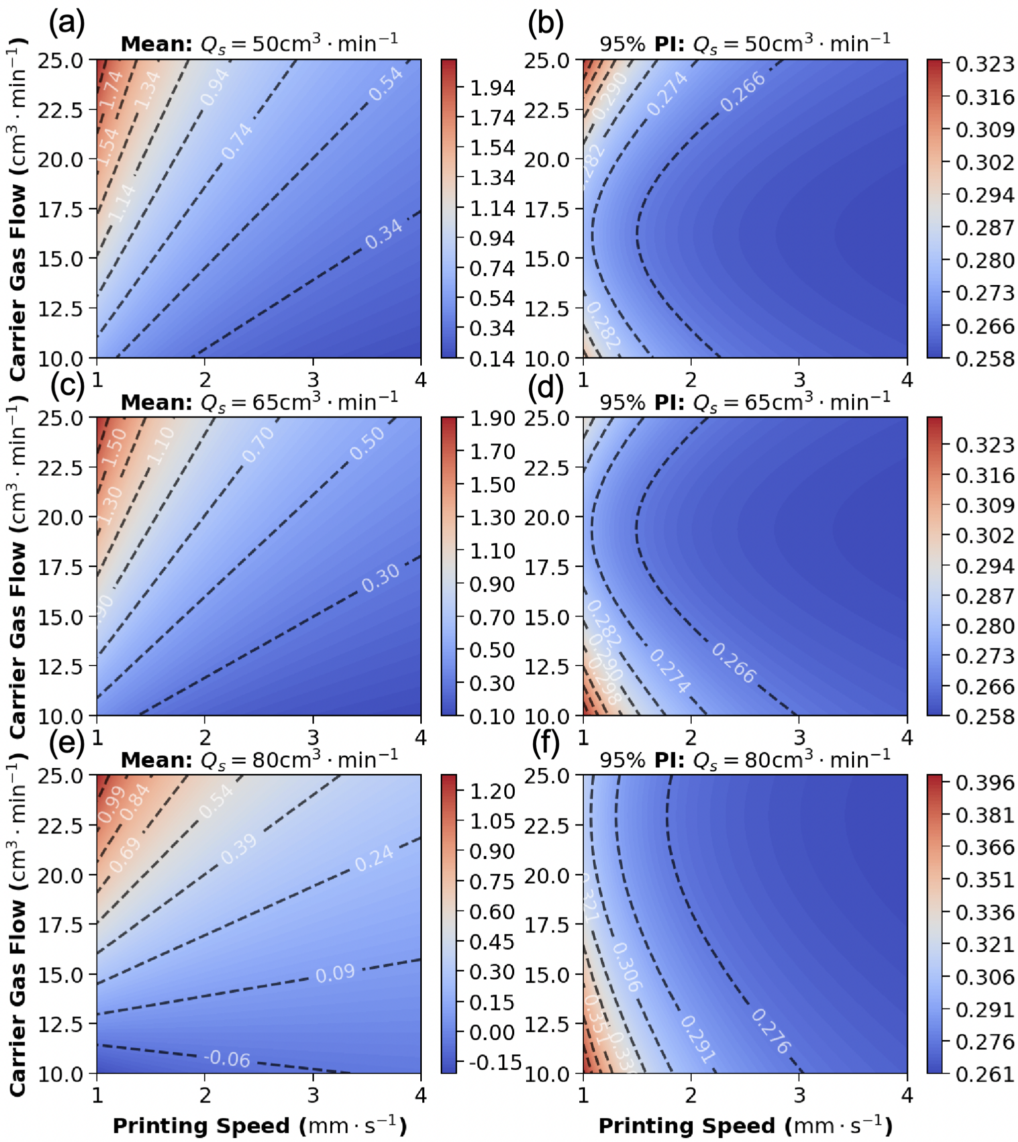

Figure C.12. This heatmap facilities inverse thickness control with $U = 45$ V using model 5. The first column is the mean prediction and the second column is the corresponding 95% PI.

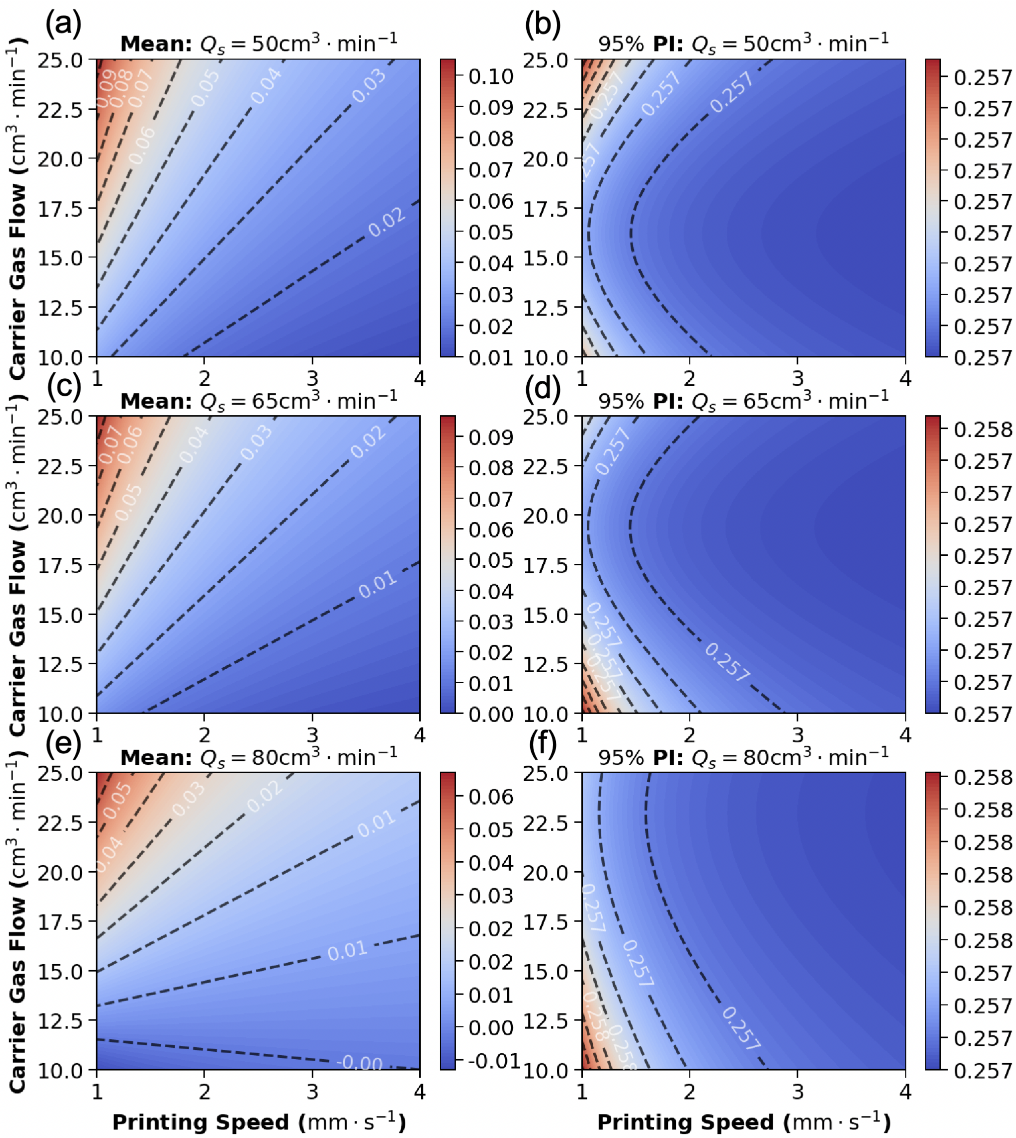

Figure C.13. This heatmap facilities inverse thickness control with $U = 20$ V using model 5. The first column is the mean prediction and the second column is the corresponding 95% PI.

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