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Unlocking insights into battery systems: A data science approach to impedance analysis

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University of Washington, Seattle

Department of Chemical Engineering and Clean Energy Institute

Monday, 29 May 2017

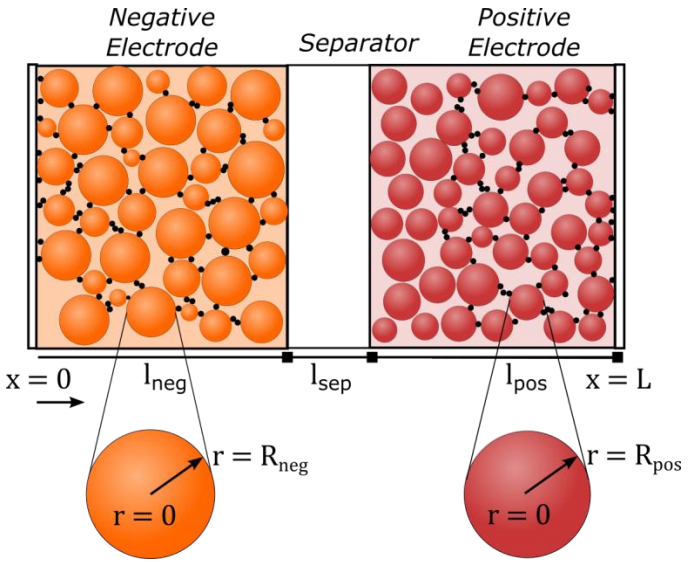
231st ECS Meeting, New Orleans, LA

Physics-based battery modeling captures complex interactions

Pseudo 2-Dimensional (P2D) model

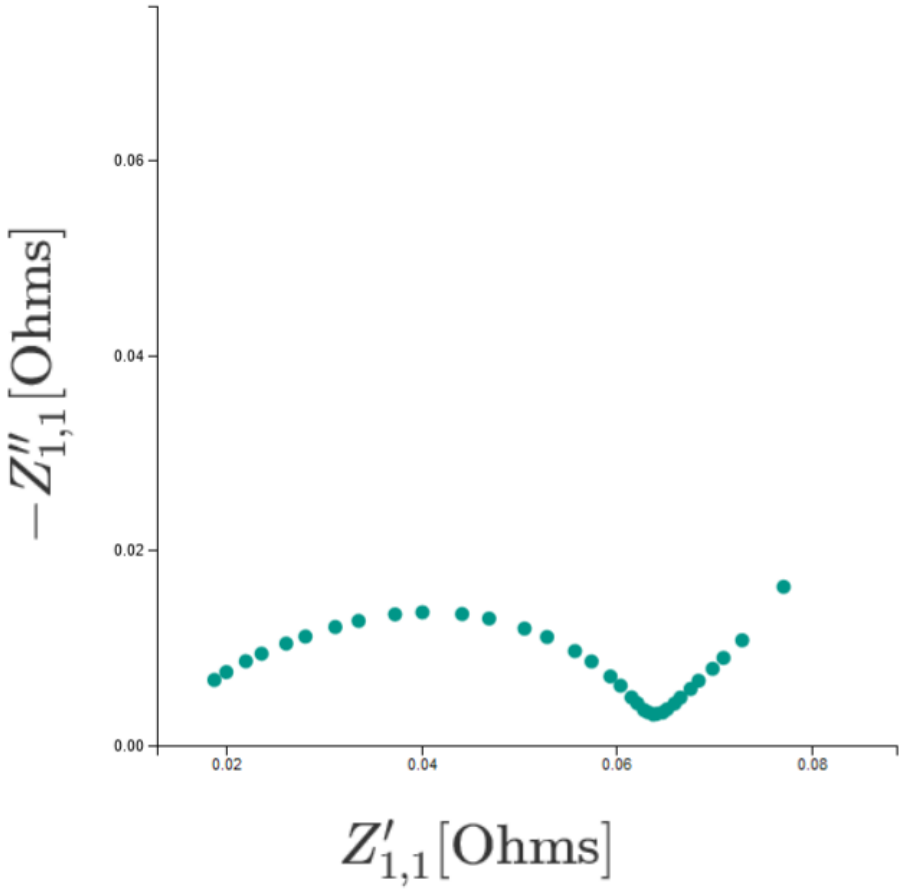
- 3 of the top 10 most cited articles in *J. Electrochem. Soc.*

Represents the interacting dynamics of the battery's **kinetics**, **mass-transport**, and **thermodynamics**



2. M. Doyle, T. F. Fuller, and J. Newman, *J. Electrochem. Soc.*, **140**, 1526–1533 (1993).
6. T. F. Fuller, M. Doyle, and J. Newman , *J. Electrochem. Soc.*, **141**, 1–10 (1994).
9. M. Doyle, J. Newman, A. S. Gozdz, C. N. Schmutz, and J.-M. Tarascon , *J. Electrochem. Soc.*, **143**, 1890–1903 (1996).

Electrochemical Impedance Spectroscopy (EIS)



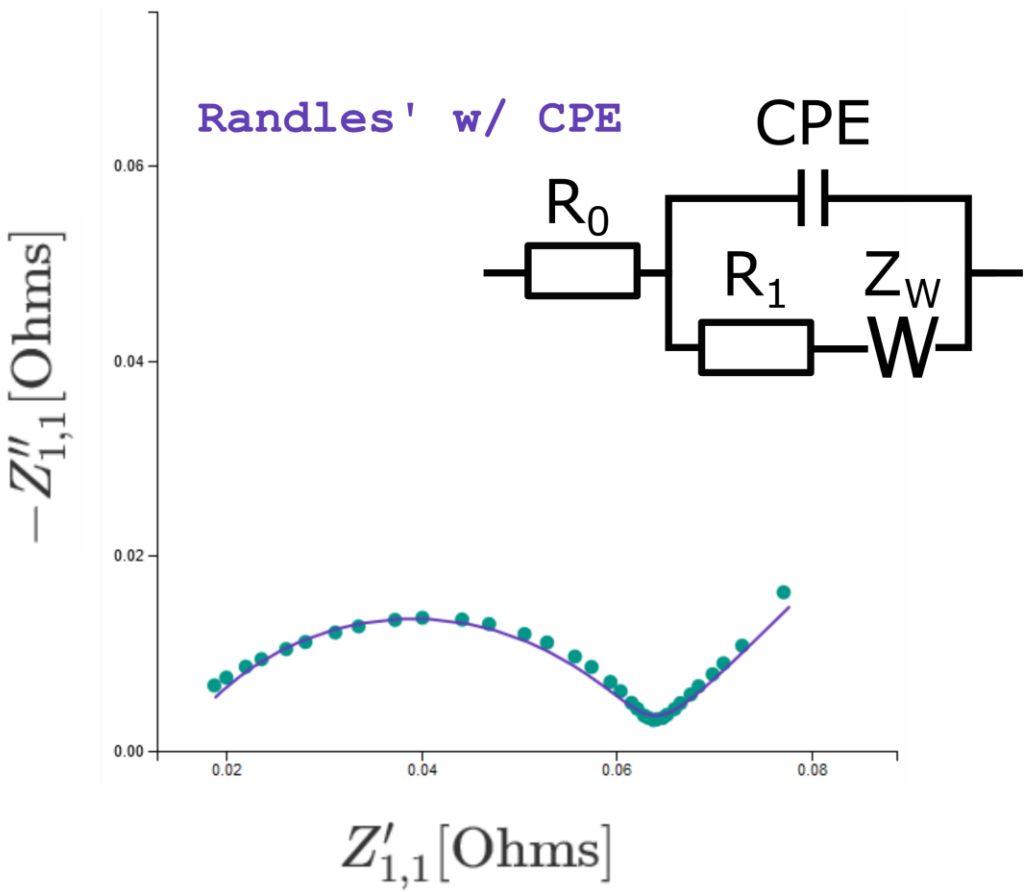
How many of you in here have used:

a physics-based model to extract parameters from an EIS spectrum?

an equivalent circuit?

Data from CALCE Battery Data Archive
http://www.calce.umd.edu/batteries/data/

Electrochemical Impedance Spectroscopy (EIS)



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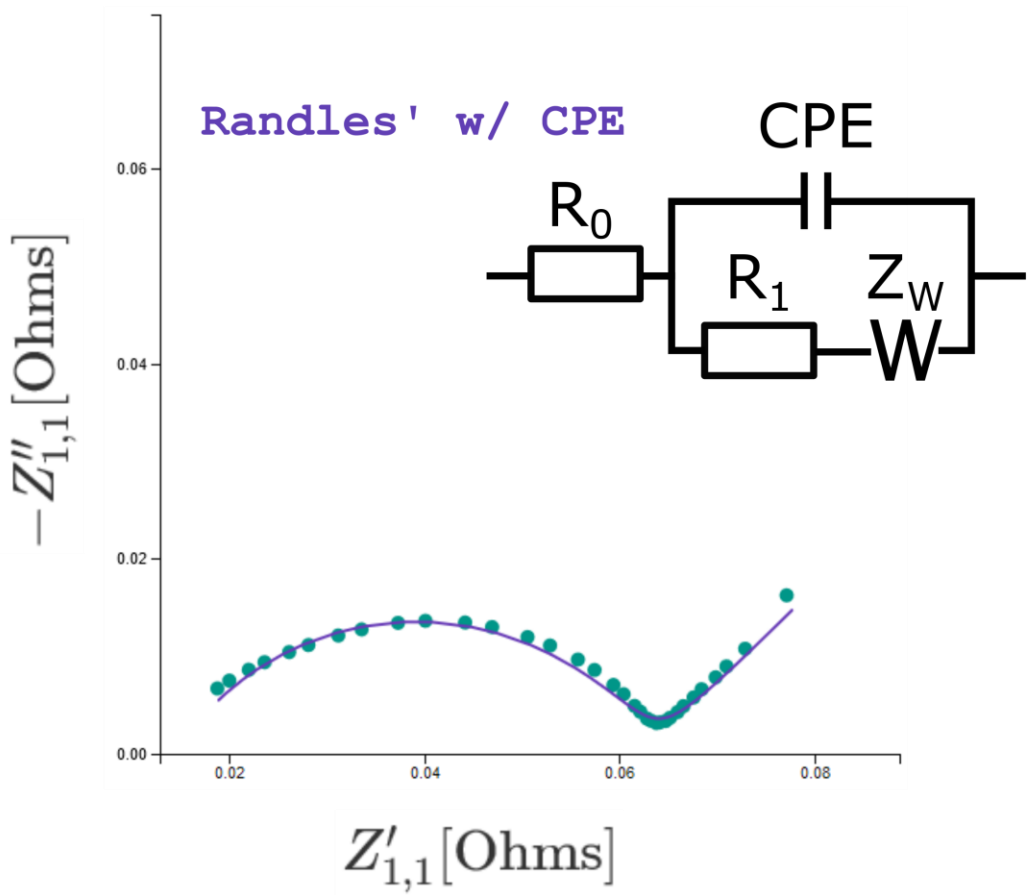

Parameter Estimates

Randles w/CPE

Parameter	Units	Best Estimate
R_0	$Ohms$	0.01429
R_1	$Ohms$	0.04879
E_1	F	0.3457
E_2	–	0.6416
W_1	$Ohms$	0.09827
W_2	Sec	284.5

Data from CALCE Battery Data Archive
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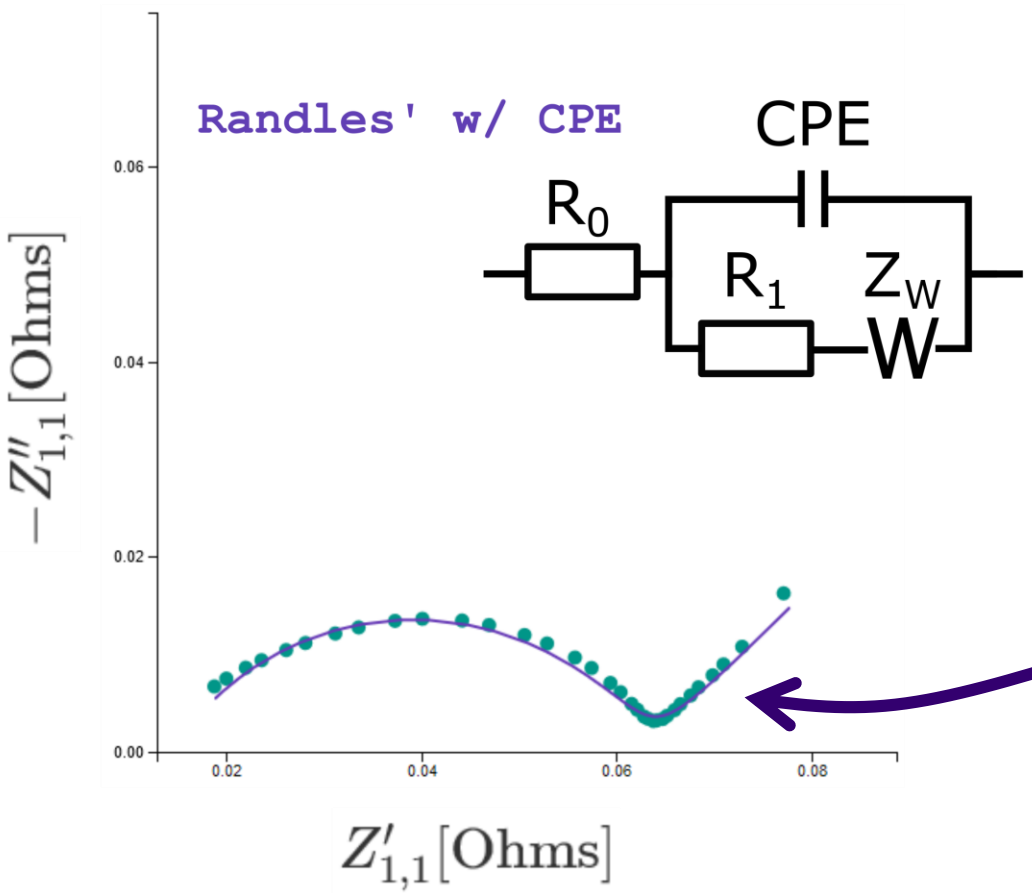
Electrochemical Impedance Spectroscopy (EIS)



Doyle et al. (2000)
Warburg element valid?

W_1	*Ohms*	0.09827
W_2	*Sec*	284.5

Data from CALCE Battery Data Archive
http://www.calce.umd.edu/batteries/data/

Physics-based impedance modeling

- A handful of in-depth applications of the P2D model to understand EIS spectra

Doyle et al. (2000) & Guo et al. (2002) – Diffusion

Dees et al. (2007) & Abraham et al. (2008) – NCA electrodes

Sikha and White (2007, 2008) – Analytical Solution

M. Doyle, J. P. Meyers, and J. Newman, *J. Electrochem. Soc.*, **147**, 99–110 (2000)
Q. Guo, V. R. Subramanian, J. W. Weidner, and R. E. White, *J. Electrochem. Soc.*, **149**, A307 (2002)
G. Sikha and R. E. White, *Journal of The Electrochemical Society*, **155**, A893 (2008)
D. P. Abraham, S. Kawauchi, and D. W. Dees, *Electrochimica Acta*, **53**, 2121–2129 (2008)

Physics-based impedance modeling

- A handful of in-depth applications of the P2D model to understand EIS spectra

Doyle et al. (2000) & Guo et a

Dees et al. (2007) & Abrahar

Sikha and White (2008) – Ar

$$\begin{bmatrix} \bar{\bar{c}}_i \\ \bar{\bar{\eta}}_i \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \dfrac{\bar{s}_i - \lambda_{1,i}}{\Theta_{1,i}} & \dfrac{\bar{s}_i - \lambda_{2,i}}{\Theta_{1,i}} \end{bmatrix} \times \begin{bmatrix} C_{1,i} \cosh \sqrt{\lambda_{1,i}}\bar{x}_i + C_{2,i} \sinh \sqrt{\lambda_{1,i}}\bar{x}_i \\ C_{3,i} \cosh \sqrt{\lambda_{2,i}}\bar{x}_i + C_{4,i} \sinh \sqrt{\lambda_{2,i}}\bar{x}_i \end{bmatrix}, \quad i = \text{a,c} \quad [4]$$

where $\lambda_{1,i}$ and $\lambda_{2,i}$ are the eigenvalues given as

$$\lambda_{1,i} = \frac{1}{2}(\bar{s}_i + \Theta_{1,i} + \Theta_{2,i} + \sqrt{\bar{s}_i^2 + 2\Theta_{1,i}\bar{s}_i - 2\Theta_{2,i}\bar{s}_i + \Theta_{1,i}^2 + \Theta_{1,i}\Theta_{2,i} + \Theta_{2,i}^2}), \quad i = \text{a,c}$$

pos

$$\lambda_{2,i} = \frac{1}{2}(\bar{s}_i + \Theta_{1,i} + \Theta_{2,i} - \sqrt{\bar{s}_i^2 + 2\Theta_{1,i}\bar{s}_i - 2\Theta_{2,i}\bar{s}_i + \Theta_{1,i}^2 + \Theta_{1,i}\Theta_{2,i} + \Theta_{2,i}^2}), \quad i = \text{a,c} \quad [5]$$

M. Doyle, J. P.)0)
Q. Guo, V. R. Subramanian, J. W)2)
G. Sikha and R. E)8)
D. P. Abraham, S. Kawa)8)

G. Sikha and R. E. White, *Journal of The Electrochemical Society*, **155**, A893 (2008).

Physics-based impedance modeling

- A handful of in-depth applications of the P2D model to understand EIS spectra

Doyle et al. (

Dees et al. (

Sikha and W

after algebraic simplification are given as follows

$$\tilde{\Phi}_{1,a}|_{\bar{x}_a=0} = -\frac{L_a^3 a_a F \beta_a}{\sigma_a^{eff^2}}\left(\frac{\bar{s}_a - \lambda_{1,a}}{\Theta_{1,a}\lambda_{1,a}}C_{1,a} + \frac{\bar{s}_a - \lambda_{2,a}}{\Theta_{1,a}\lambda_{2,a}}C_{3,a}\right) + C_{8,a} \quad [30]$$

$$\tilde{\Phi}_{1,c}|_{\bar{x}_c=1} = \frac{L_c^3 a_c F \beta_c}{\sigma_c^{eff^2}}\left[\frac{\bar{s}_c - \lambda_{1,c}}{\Theta_{1,c}\lambda_{1,c}}(C_{1,c}\cosh\sqrt{\lambda_{1,c}} + C_{2,c}\sinh\sqrt{\lambda_{1,c}}) \quad C_{2,i}\sinh\sqrt{\lambda_{1,i}}\bar{x}_i\right], \quad i = a,c \; [4]$$

$$+ \frac{\bar{s}_c - \lambda_{2,c}}{\Theta_{1,c}\lambda_{2,c}}(C_{3,c}\cosh\sqrt{\lambda_{2,c}} + C_{4,c}\sinh\sqrt{\lambda_{2,c}})\Big] + C_{7,c} \quad C_{4,i}\sinh\sqrt{\lambda_{2,i}}\bar{x}_i$$

es given as

$$+ C_{8,c} \quad [31]$$

$$+ \sqrt{\bar{s}_i^2 + 2\Theta_{1,i}\bar{s}_i - 2\Theta_{2,i}\bar{s}_i + \Theta_{1,i}^2 + \Theta_{1,i}\Theta_{2,i} + \Theta_{2,i}^2}), \quad i = a,c$$

pos

$$\lambda_{2,i} = \frac{1}{2}(\bar{s}_i + \Theta_{1,i} + \Theta_{2,i}$$

$$- \sqrt{\bar{s}_i^2 + 2\Theta_{1,i}\bar{s}_i - 2\Theta_{2,i}\bar{s}_i + \Theta_{1,i}^2 + \Theta_{1,i}\Theta_{2,i} + \Theta_{2,i}^2}), \quad i = a,c \quad [5]$$

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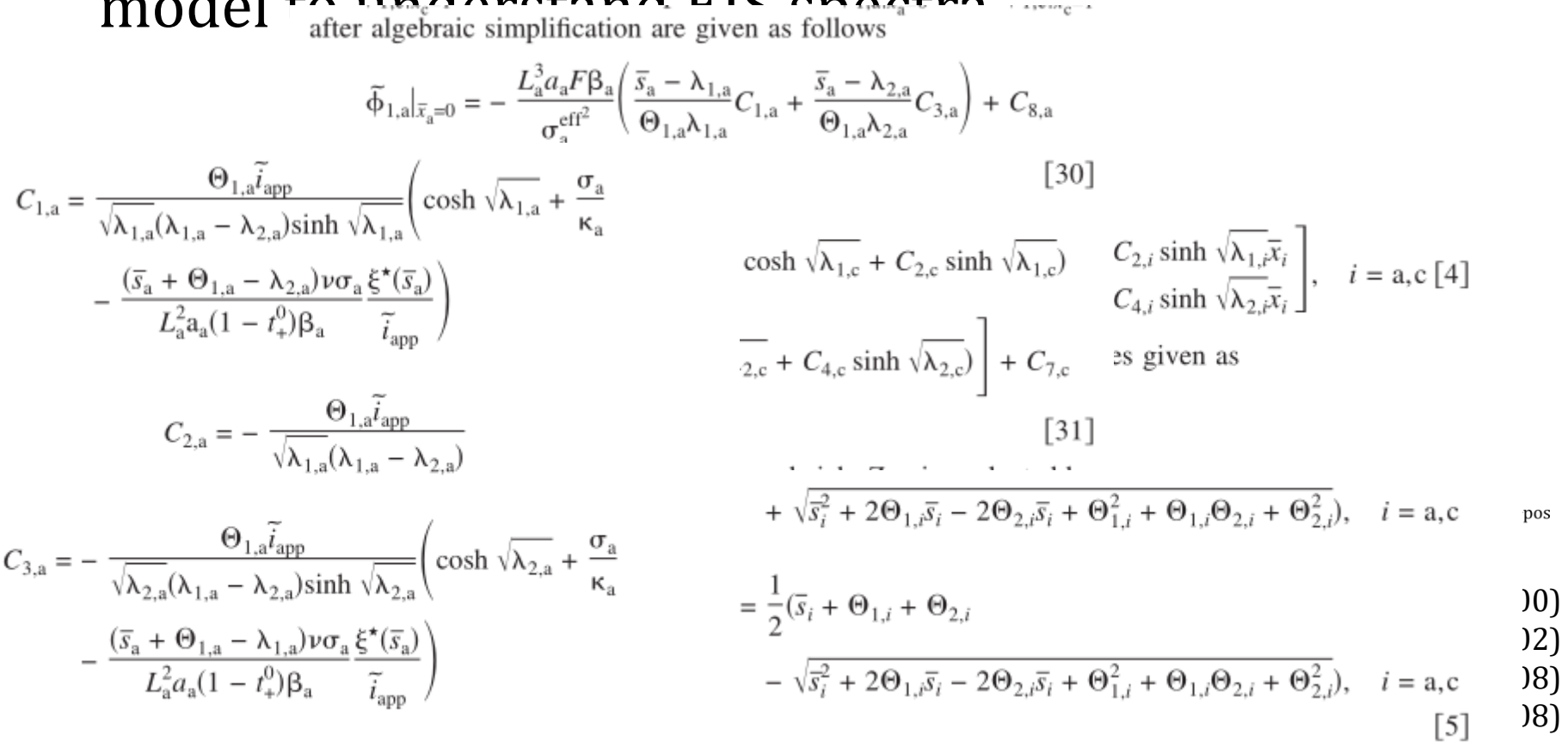
Physics-based impedance modeling

- A handful of in-depth applications of the P2D model to understand EIS spectra



after algebraic simplification are given as follows

$$\tilde{\Phi}_{1,a}\big|_{\bar{x}_a=0} = -\frac{L_a^3 a_a F \beta_a}{\sigma_a^{eff2}}\left(\frac{\bar{s}_a - \lambda_{1,a}}{\Theta_{1,a}\lambda_{1,a}}C_{1,a} + \frac{\bar{s}_a - \lambda_{2,a}}{\Theta_{1,a}\lambda_{2,a}}C_{3,a}\right) + C_{8,a} \quad [30]$$

$$C_{1,a} = \frac{\Theta_{1,a}\tilde{i}_{app}}{\sqrt{\lambda_{1,a}}(\lambda_{1,a}-\lambda_{2,a})\sinh\sqrt{\lambda_{1,a}}}\left(\cosh\sqrt{\lambda_{1,a}} + \frac{\sigma_a}{\kappa_a} - \frac{(\bar{s}_a + \Theta_{1,a} - \lambda_{2,a})\nu\sigma_a}{L_a^2 a_a(1-t_+^0)\beta_a}\frac{\xi^\star(\bar{s}_a)}{\tilde{i}_{app}}\right)$$

$$C_{2,a} = -\frac{\Theta_{1,a}\tilde{i}_{app}}{\sqrt{\lambda_{1,a}}(\lambda_{1,a}-\lambda_{2,a})}$$

$$C_{3,a} = -\frac{\Theta_{1,a}\tilde{i}_{app}}{\sqrt{\lambda_{2,a}}(\lambda_{1,a}-\lambda_{2,a})\sinh\sqrt{\lambda_{2,a}}}\left(\cosh\sqrt{\lambda_{2,a}} + \frac{\sigma_a}{\kappa_a} - \frac{(\bar{s}_a + \Theta_{1,a} - \lambda_{1,a})\nu\sigma_a}{L_a^2 a_a(1-t_+^0)\beta_a}\frac{\xi^\star(\bar{s}_a)}{\tilde{i}_{app}}\right)$$

$$\cosh\sqrt{\lambda_{1,c}} + C_{2,c}\sinh\sqrt{\lambda_{1,c}}) \quad C_{2,i}\sinh\sqrt{\lambda_{1,i}}\bar{x}_i$$
$$C_{4,i}\sinh\sqrt{\lambda_{2,i}}\bar{x}_i\Big], \quad i = a,c \; [4]$$

$$\overline{{}_{2,c}} + C_{4,c}\sinh\sqrt{\lambda_{2,c}})\Big] + C_{7,c} \quad \text{es given as}$$

[31]

$$+\sqrt{\bar{s}_i^2 + 2\Theta_{1,i}\bar{s}_i - 2\Theta_{2,i}\bar{s}_i + \Theta_{1,i}^2 + \Theta_{1,i}\Theta_{2,i} + \Theta_{2,i}^2}), \quad i = a,c$$

pos

$$= \frac{1}{2}(\bar{s}_i + \Theta_{1,i} + \Theta_{2,i}$$

)0)

$$-\sqrt{\bar{s}_i^2 + 2\Theta_{1,i}\bar{s}_i - 2\Theta_{2,i}\bar{s}_i + \Theta_{1,i}^2 + \Theta_{1,i}\Theta_{2,i} + \Theta_{2,i}^2}), \quad i = a,c$$

)2)
)8)
)8)

[5]

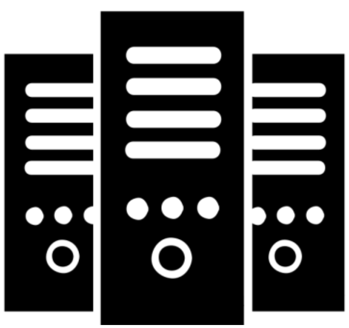
G. Sikha and R. E. White, *Journal of The Electrochemical Society*, **155**, A893 (2008).

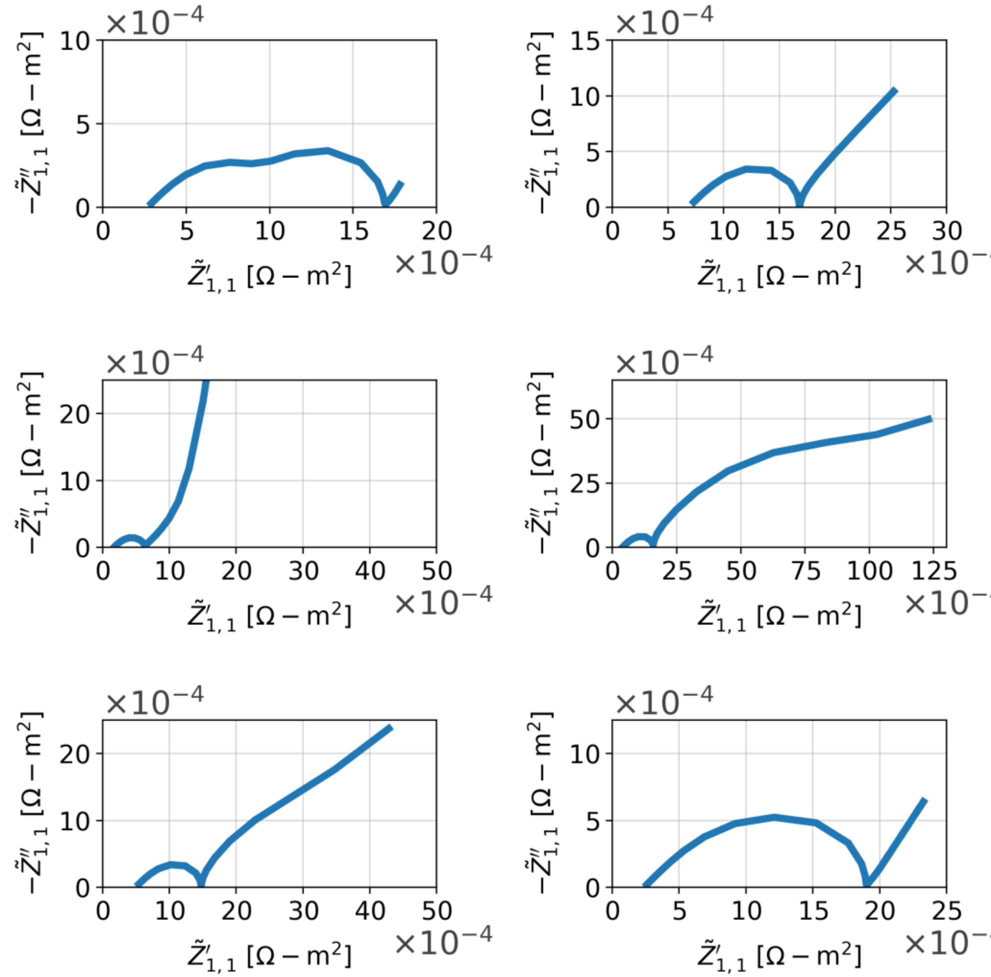
ImpedanceAnalyzer: A user centered approach

Initial dataset:

- 40,000 spectra
- 26 parameters
- Sobol' sampling

1. Generate dataset





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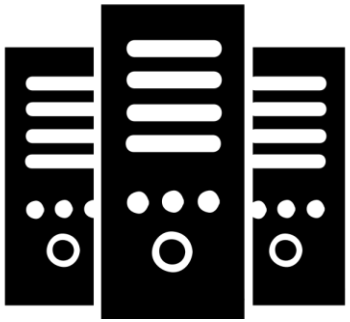
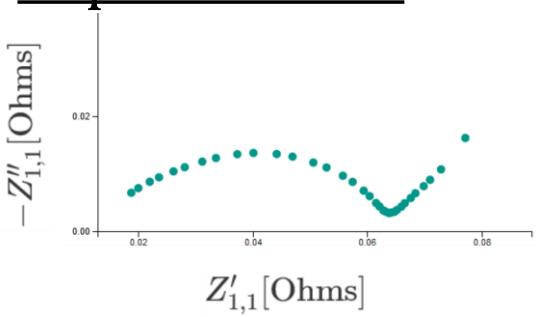
ImpedanceAnalyzer:
A user centered approach

1. Generate dataset

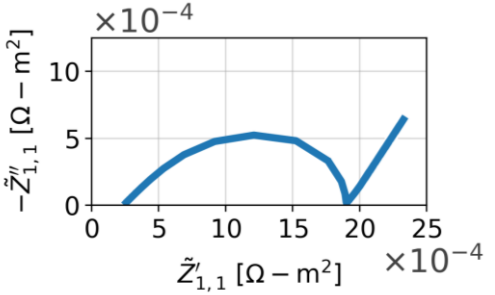


2. Find match to experimental spectra

Experimental:



Simulated:



ImpedanceAnalyzer: A user centered approach

2. Find match to experimental spectra

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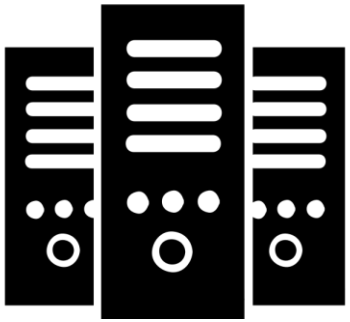
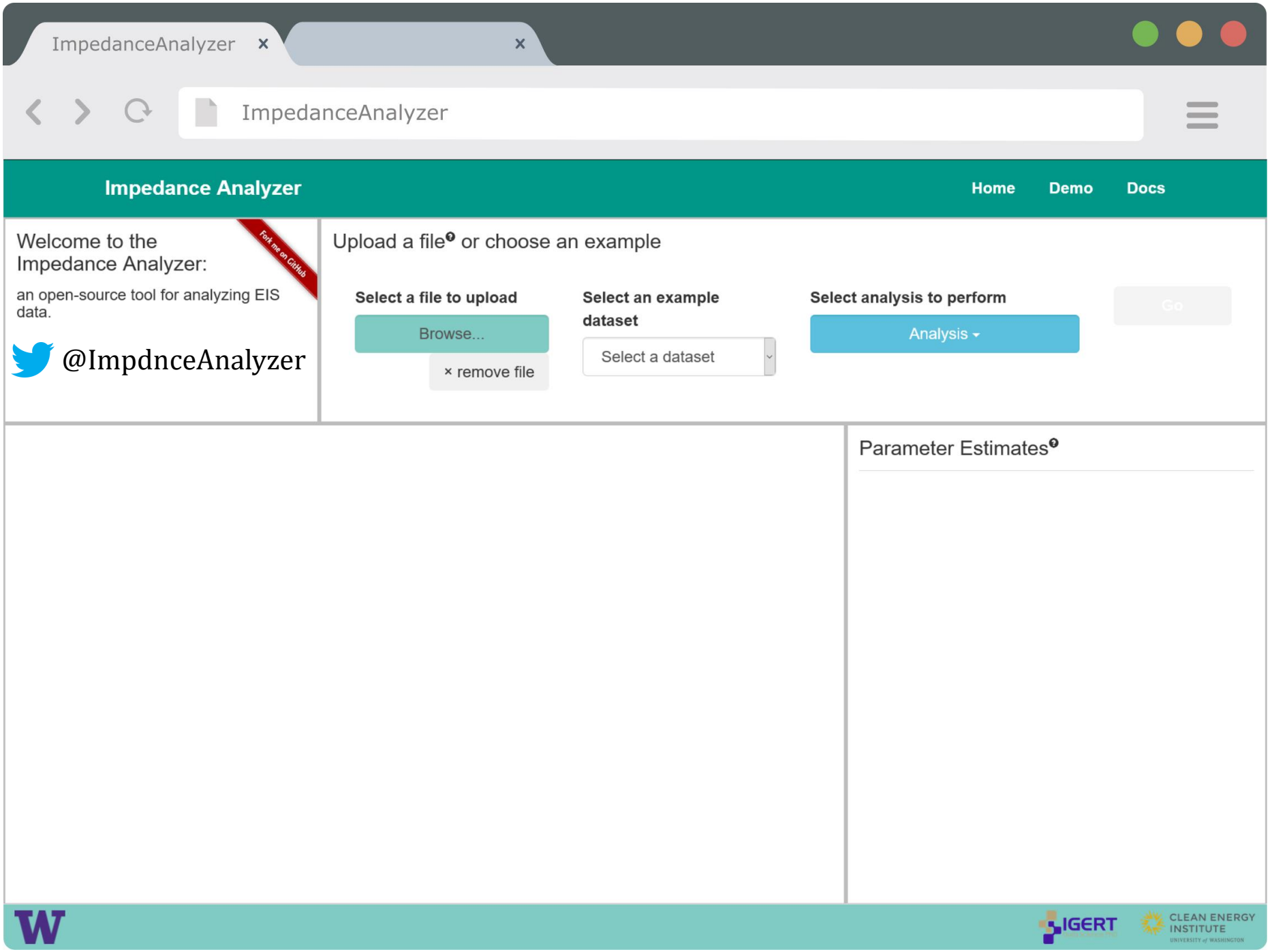


3. Visualize + Explore

Demo

Beta version

with preliminary P2D dataset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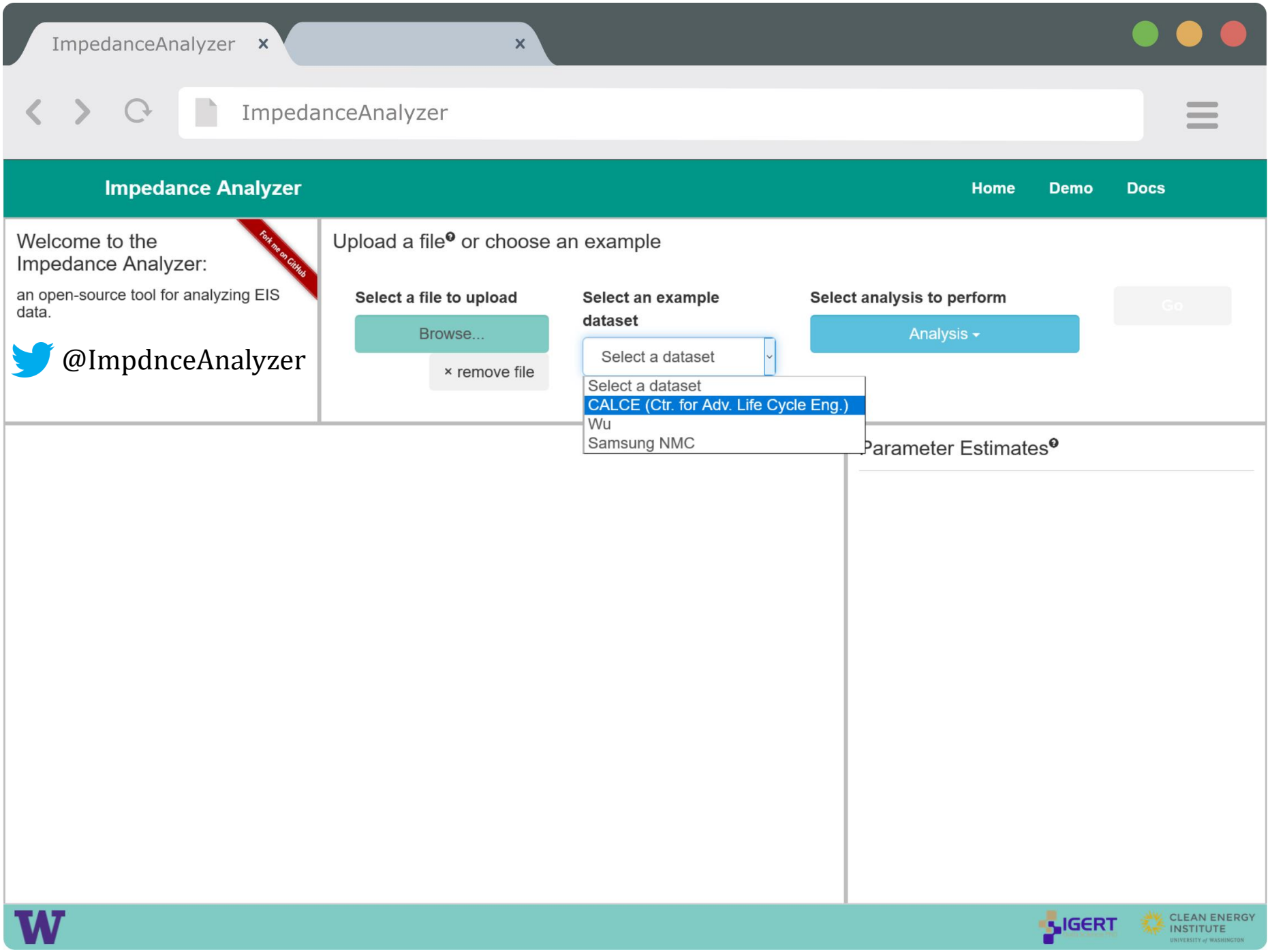
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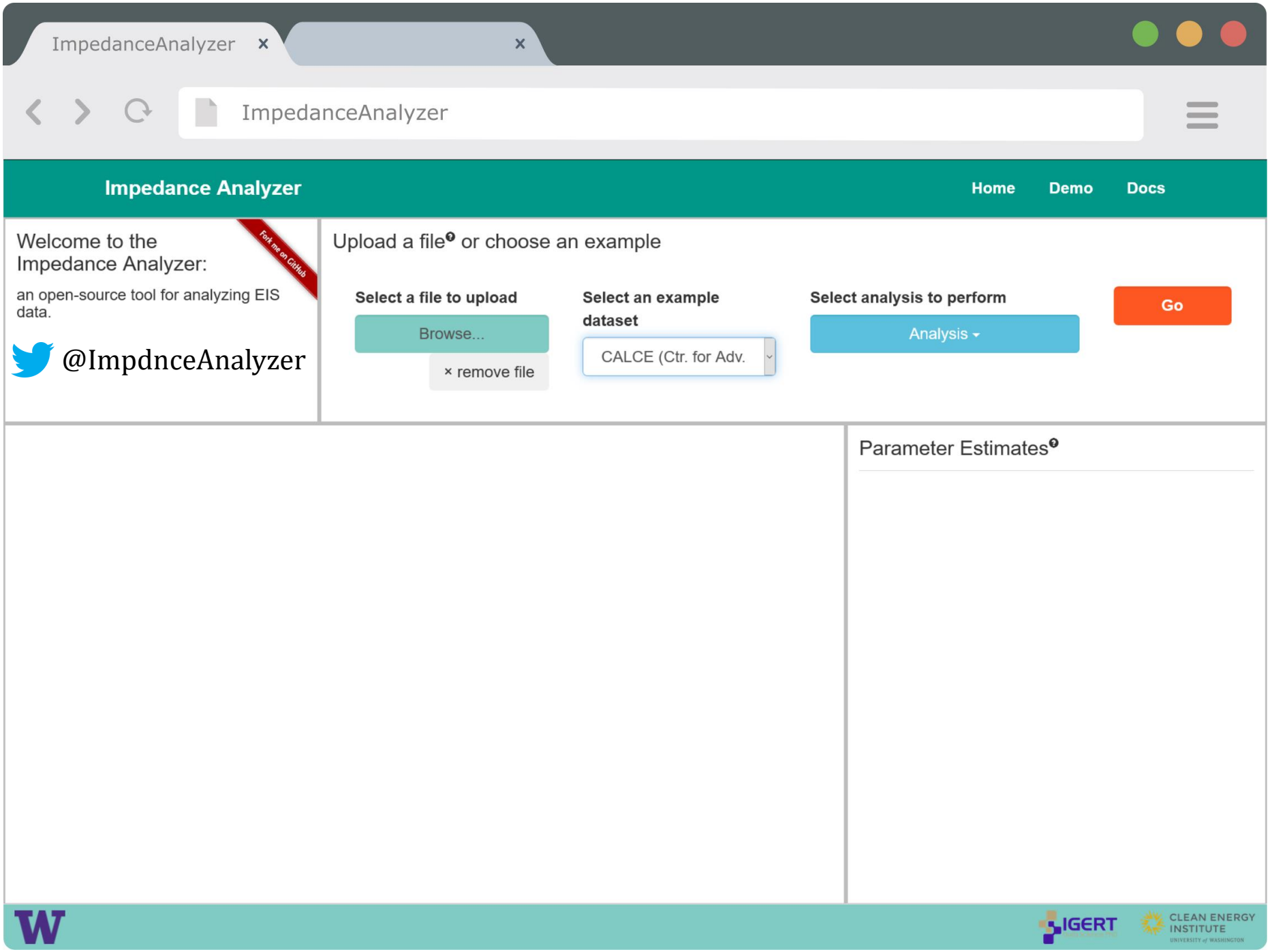
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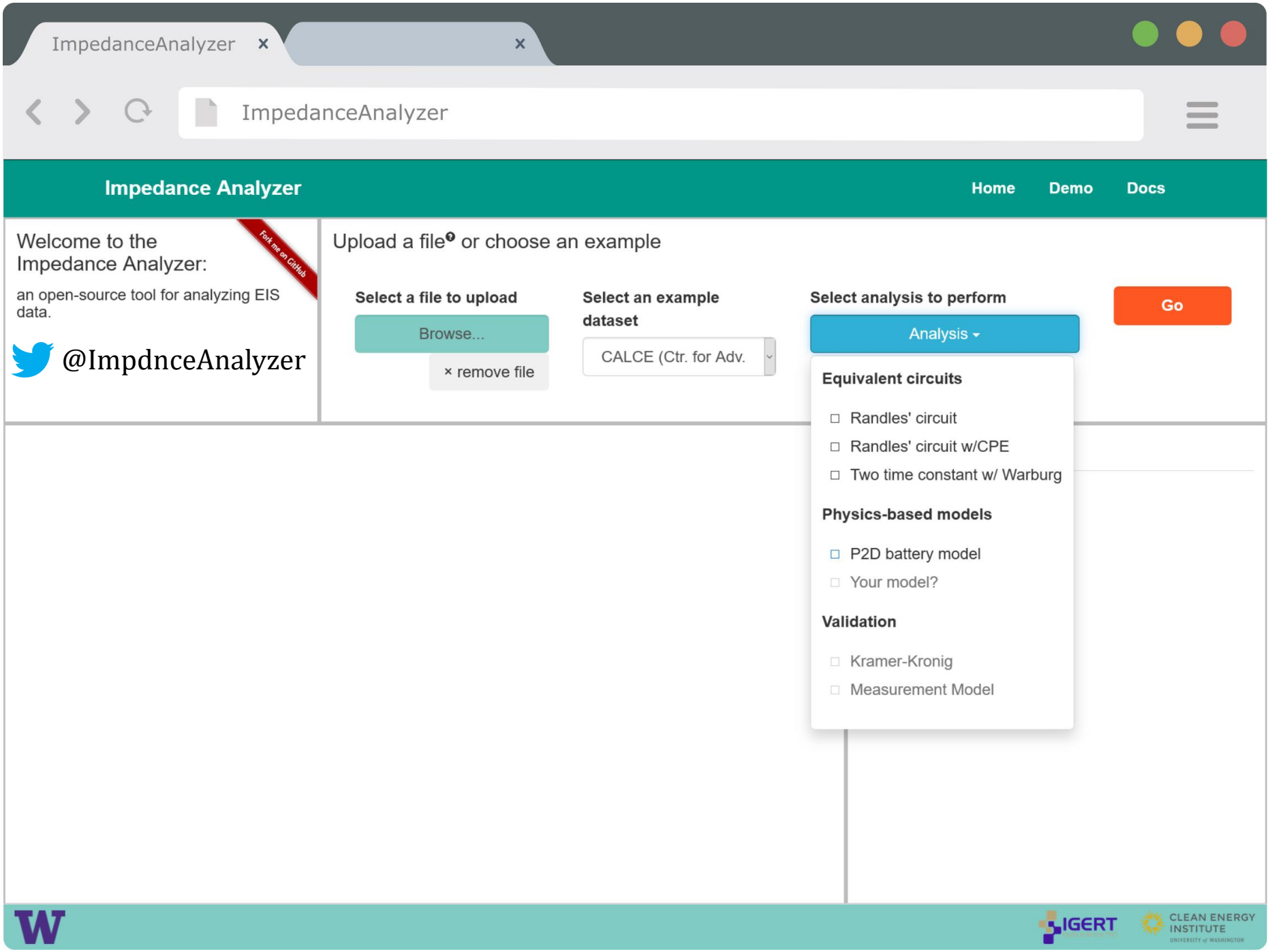
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Randles' circuit
Randles' circuit w/CPE
Two time constant w/ Warburg
Physics-based models
P2D battery model
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Validation
Kramer-Kronig
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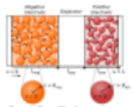
Input options for model fits



Pseudo 2-Dimensional

Select type of fit

Capacity

Capacity (mAh) mAh

Dataset: Initial 40,000 spectra

Finished

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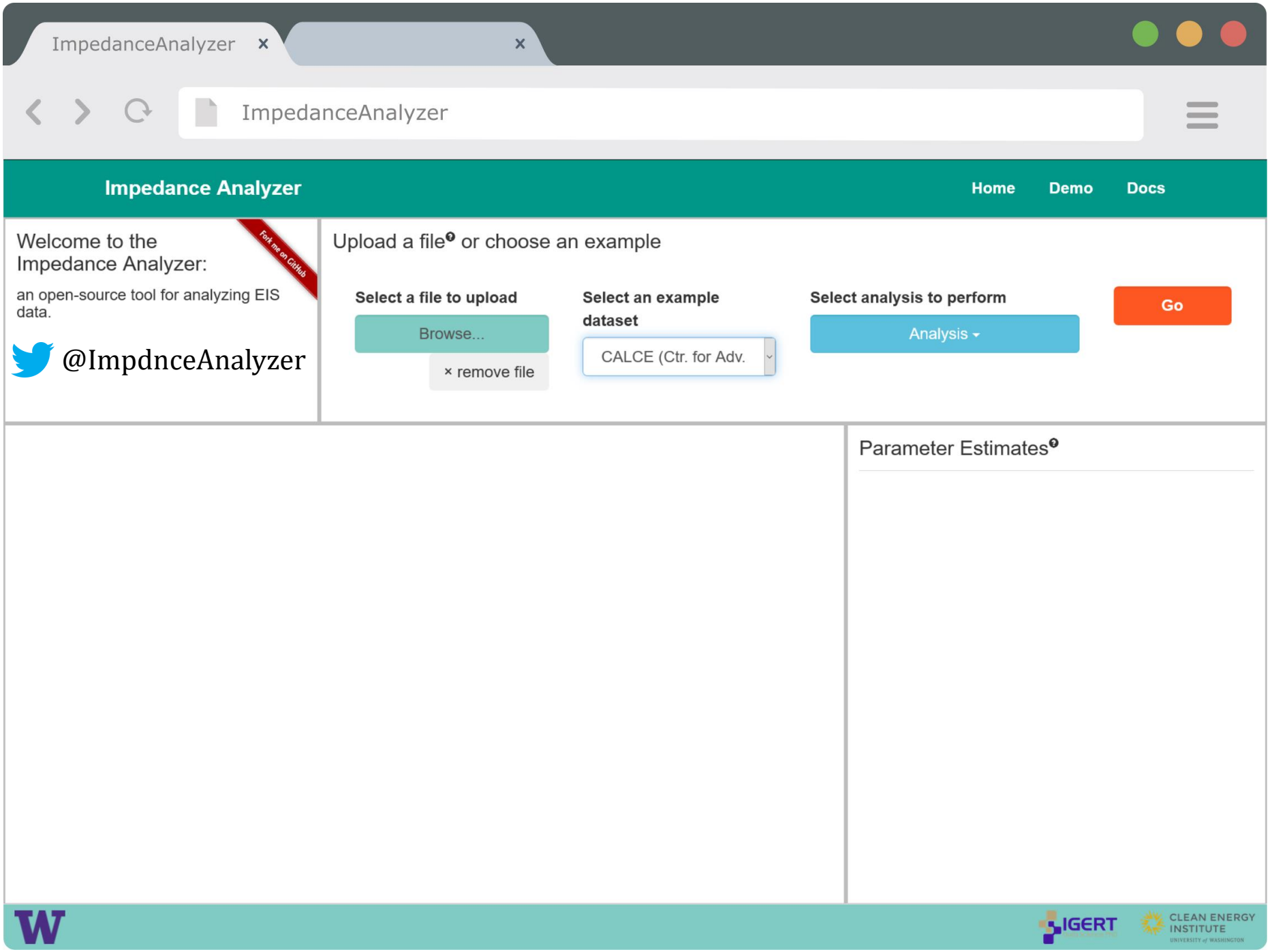
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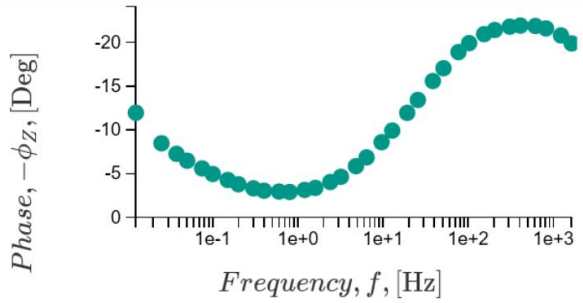

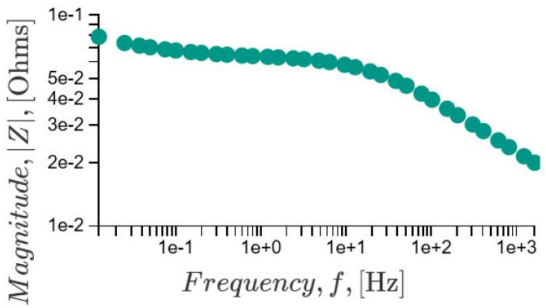

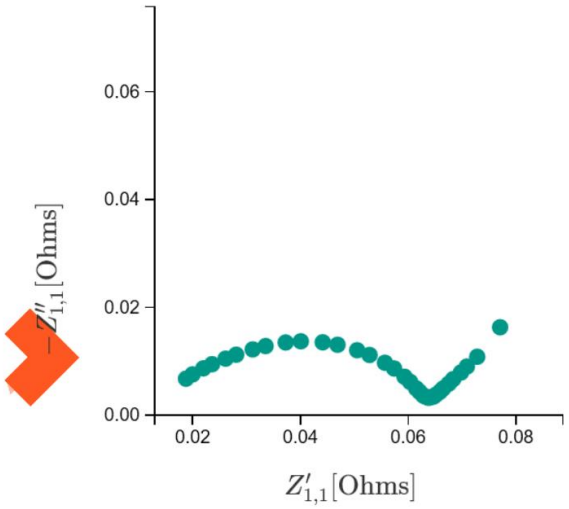

Matching...

Parameter Estimates

Download Results

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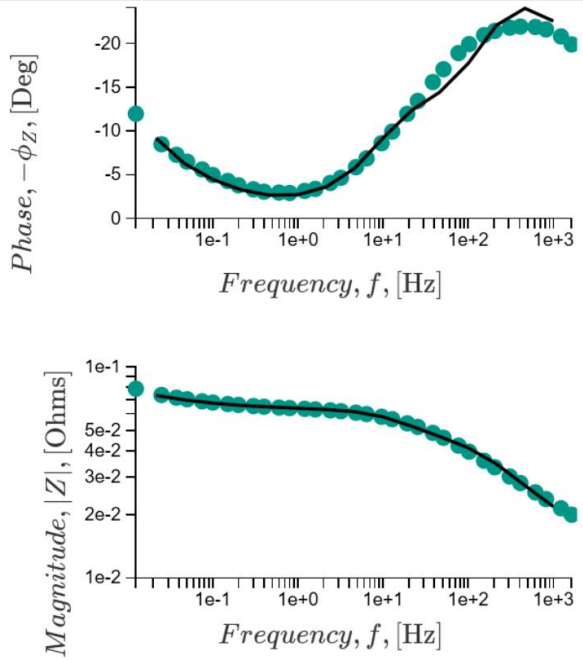

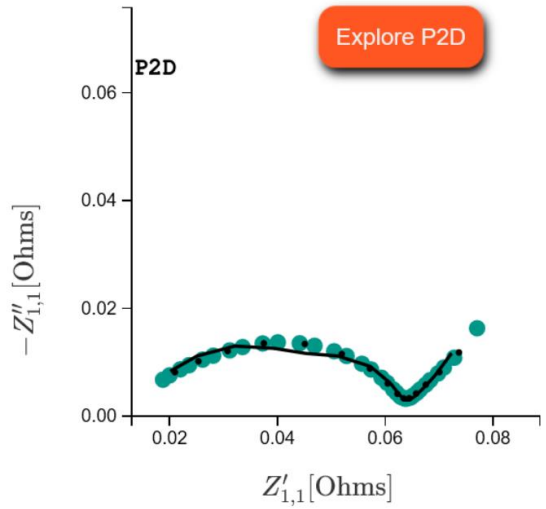

Matching completed in 7 seconds

Parameter Estimates

Download Results

P2D

Parameter	Units	Best Estimate
fit	cm^2	300.3
run	run	6230
l_{neg}	m	0.0003199
l_{sep}	m	0.00003598
l_{pos}	m	0.0001591

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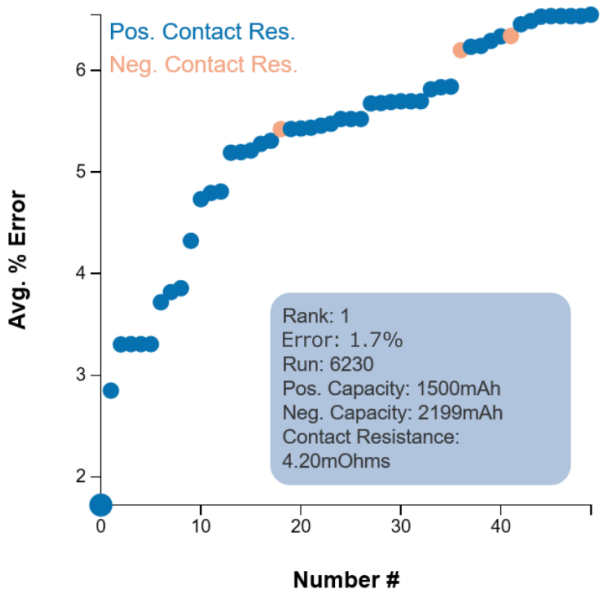
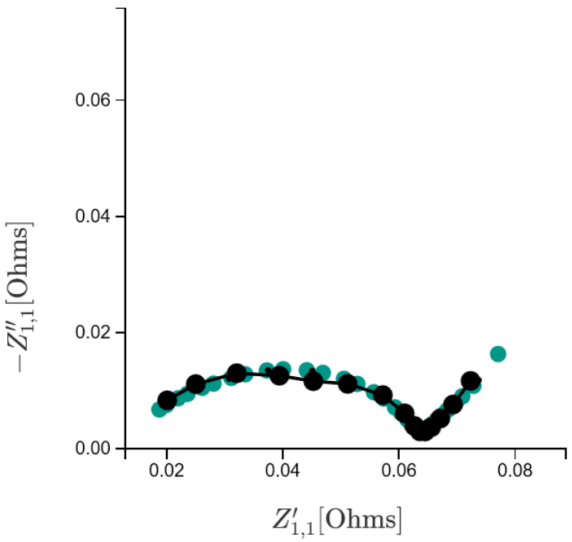
Explore P2D fit





name	units	6230
fit	cm^2	3.0032e+02
run		6230.0
l_{neg}	m	3.1993e-04
l_{sep}	m	3.5984e-05
l_{pos}	m	1.5907e-04
$R_{p,neg}$	m	1.9324e-05
$R_{p,pos}$	m	1.4990e-06
		6.1699e-02

Average % Error:

$$\frac{\sum_i^N \sqrt{\left(Z'_{model}(\omega_i) - Z'_{data}(\omega_i)\right)^2 + \left(Z''_{model}(\omega_i) - Z''_{data}(\omega_i)\right)^2}}{\sum_i^N |Z_{data}(\omega_i)|}$$

Close

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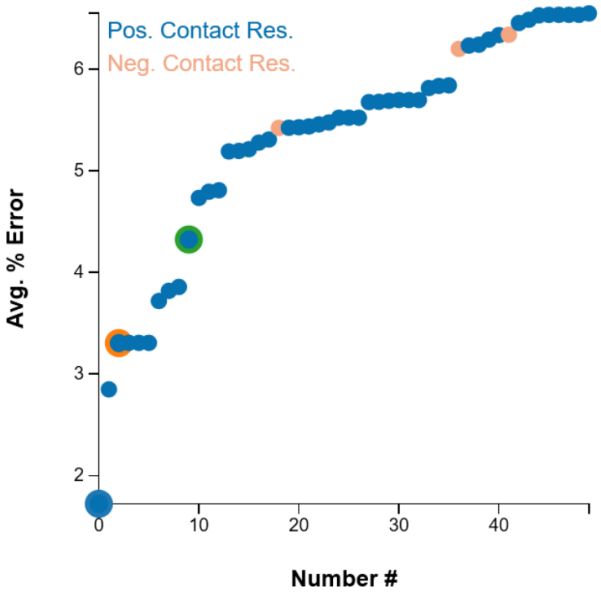
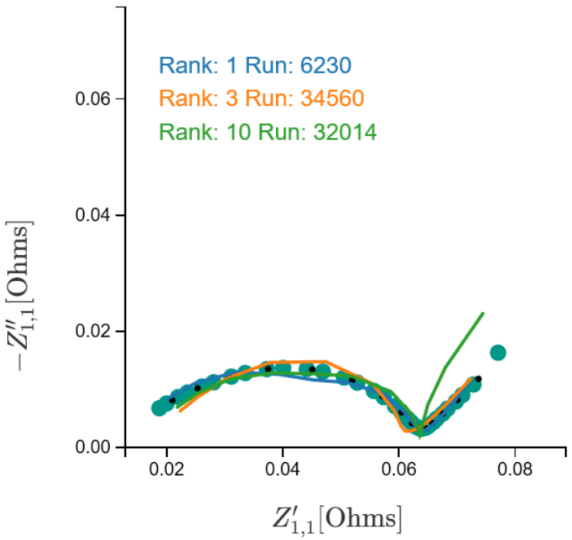
Explore P2D fit

Download Parameter Table





	6230	34560	32014
η^2	3.0032e+02	3.1388e+02	2.1835e+02
	6230.0	34560.0	32014.0
η	3.1993e-04	4.2263e-04	2.8666e-04
η	3.5984e-05	1.7852e-05	2.8352e-05
η	1.5907e-04	1.5011e-04	3.3642e-04
η	1.9324e-05	2.4471e-06	6.4176e-06
η	1.4990e-06	6.1167e-06	2.3843e-06
	6.1699e-02	9.4365e-02	6.8818e-02

Average % Error:

$$\frac{\sum_{i}^{N}\sqrt{\left(Z'_{model}(\omega_i) - Z'_{data}(\omega_i)\right)^2 + \left(Z''_{model}(\omega_i) - Z''_{data}(\omega_i)\right)^2}}{\sum_{i}^{N}|Z_{data}(\omega_i)|}$$

Close

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Summary

- With the ImpedanceAnalyzer, physics-based impedance analysis can be as easy as using an equivalent circuit
- Future improvements will include building a larger dataset and integrating local optimization
- Open-source software projects allow the ECS community to build the tools that it wants and needs

Equivalent circuits: **fast and easy to use**

Physics-based models: **+ sophisticated analysis**

ImpedanceAnalyzer

Looking for a few beta testers:

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For updates and more information…

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(slides: `mattmurbach.com/ecs2017a`)