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Data science tools for incorporating physics-based models into analysis of impedance spectra

Matthew D. Murbach and Daniel T. Schwartz

University of Washington, Seattle

Department of Chemical Engineering and Clean Energy Institute

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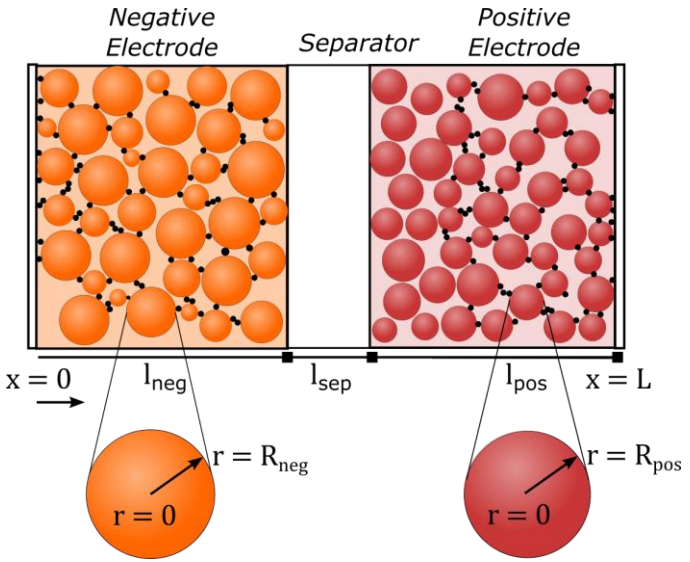
231st ECS Meeting, New Orleans, LA

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).

Many decades of embedded electrochemical knowledge

Side reactions and degradation (SEI layer)

P. Arora et al. (1998), P. Ramadass et al. (2004), etc.

Stress-strain and particle-particle interactions

R. E. García et al. (2005), D. E. Stephenson (2007), etc.

Thermal effects

M. Guo and R. E. White (2013), etc.

and others…

Limited number of physics-based impedance modeling examples

Doyle et al. (2000) & Guo et al. (2002) – Warburg element not ideal for capturing diffusion

Dees (2007) & Abraham et al. (2008) – in-depth understanding of 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)

ImpedanceAnalyzer: A user centered approach

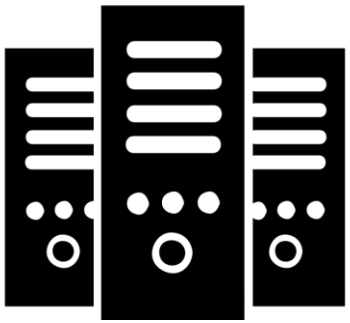
- Frequency domain formulation

$$X(\boldsymbol{x},t) = Re\{\tilde{X}(\boldsymbol{x})\exp(j\omega_1 t)\}$$

$$\tilde{X}(\boldsymbol{x}) = \tilde{X}'(\boldsymbol{x}) - j\tilde{X}''(\boldsymbol{x})$$

M.D. Murbach and D.T. Schwartz, *J. Electrochem. Soc.*, **164**, E1-E10 (2017)

1. Generate dataset



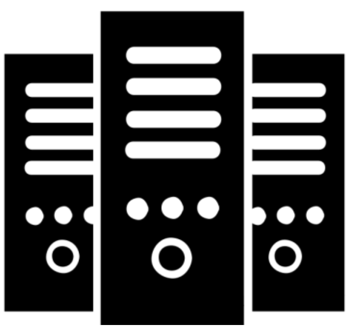
- COMSOL Multiphysics
- Tradeoffs between fast computations and numerical accuracy

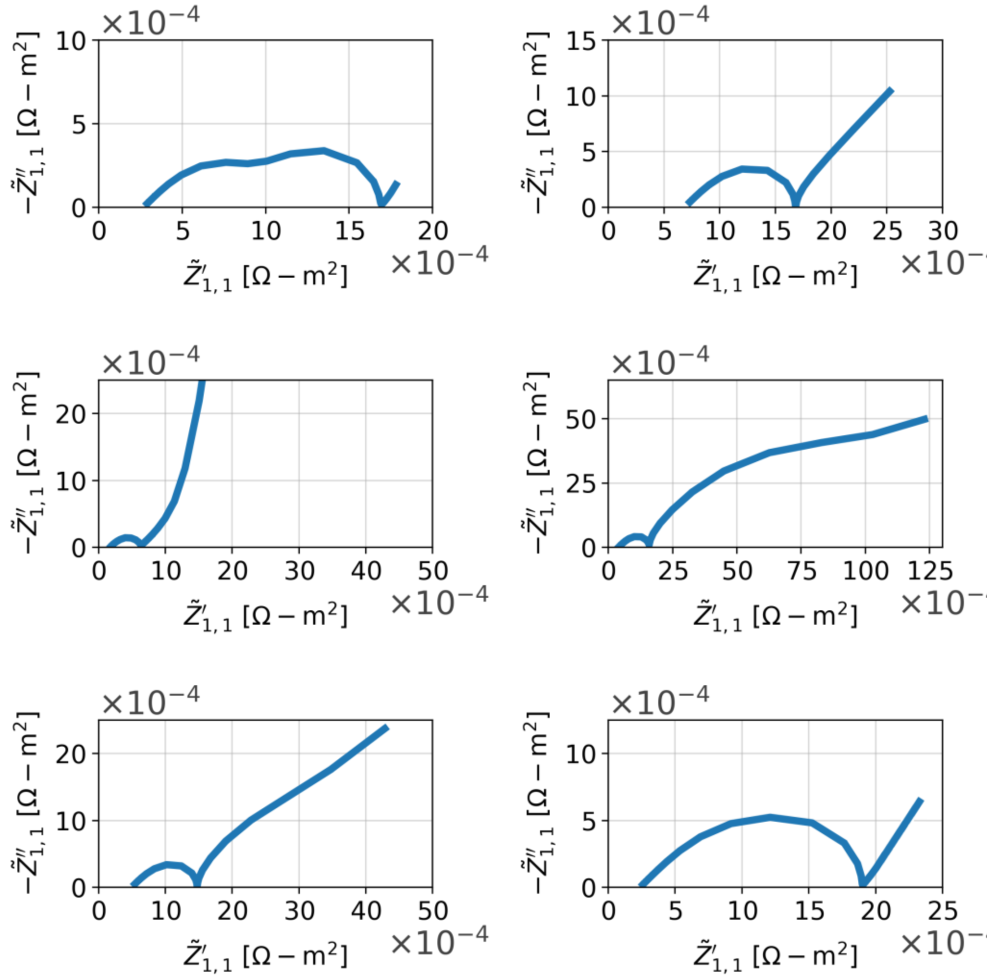
ImpedanceAnalyzer: A user centered approach

Initial dataset:

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

1. Generate dataset





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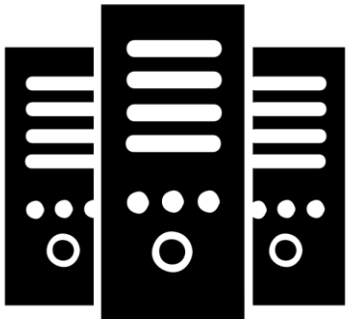
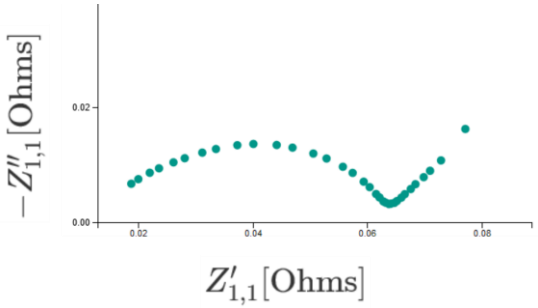
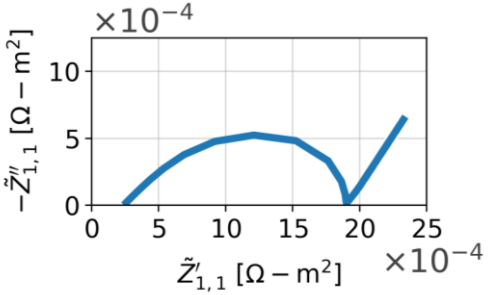


2. Find match to experimental spectra

Experimental:



Simulated:



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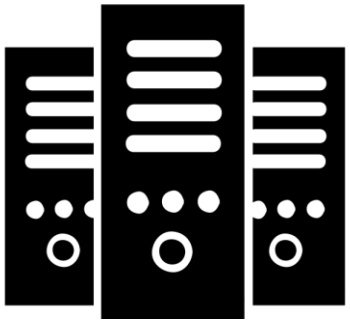
ImpedanceAnalyzer: A user centered approach

2. Find match to experimental spectra

1. Generate dataset

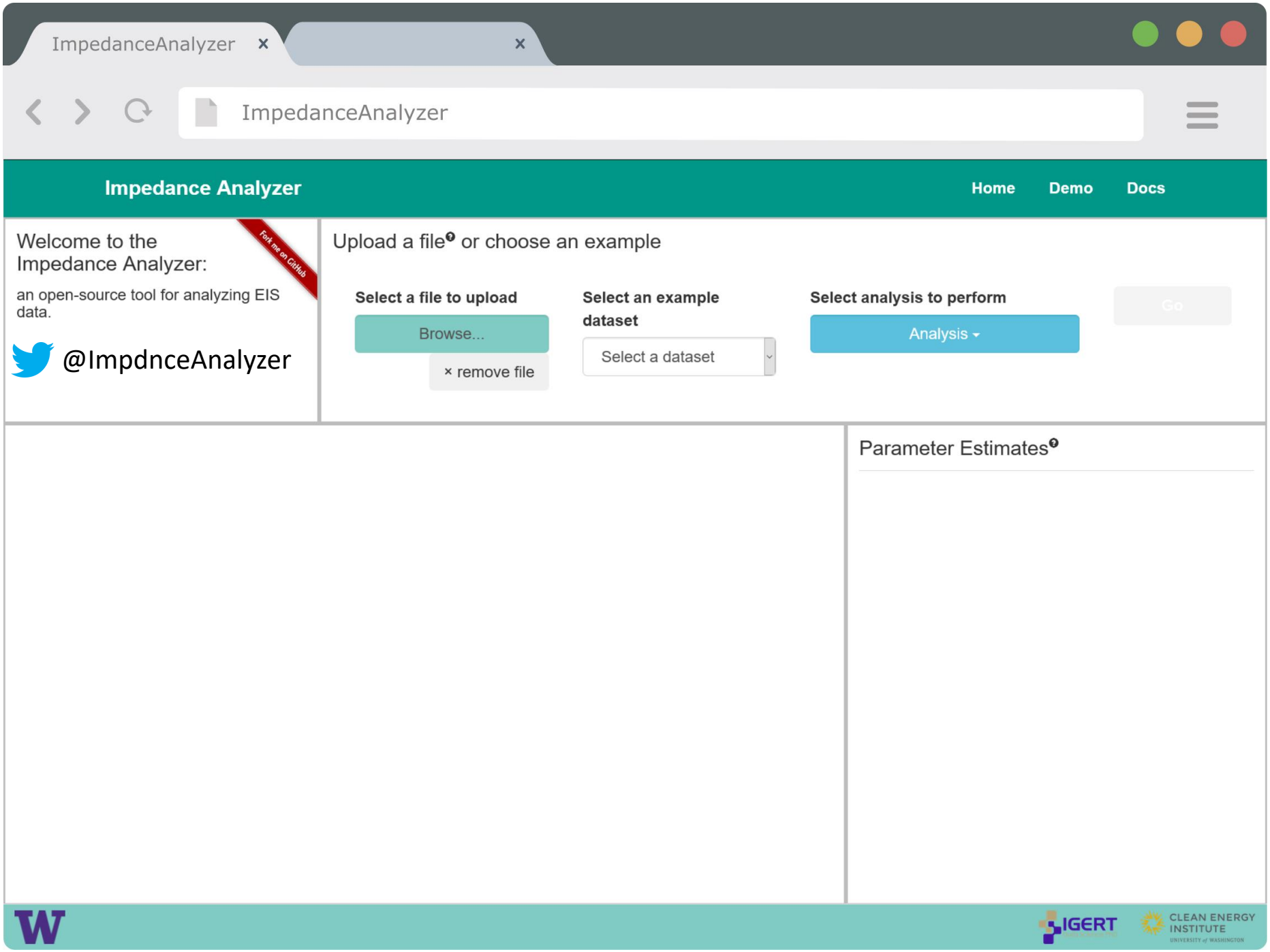


3. Visualize + Explore

Demo

Beta version

with preliminary P2D dataset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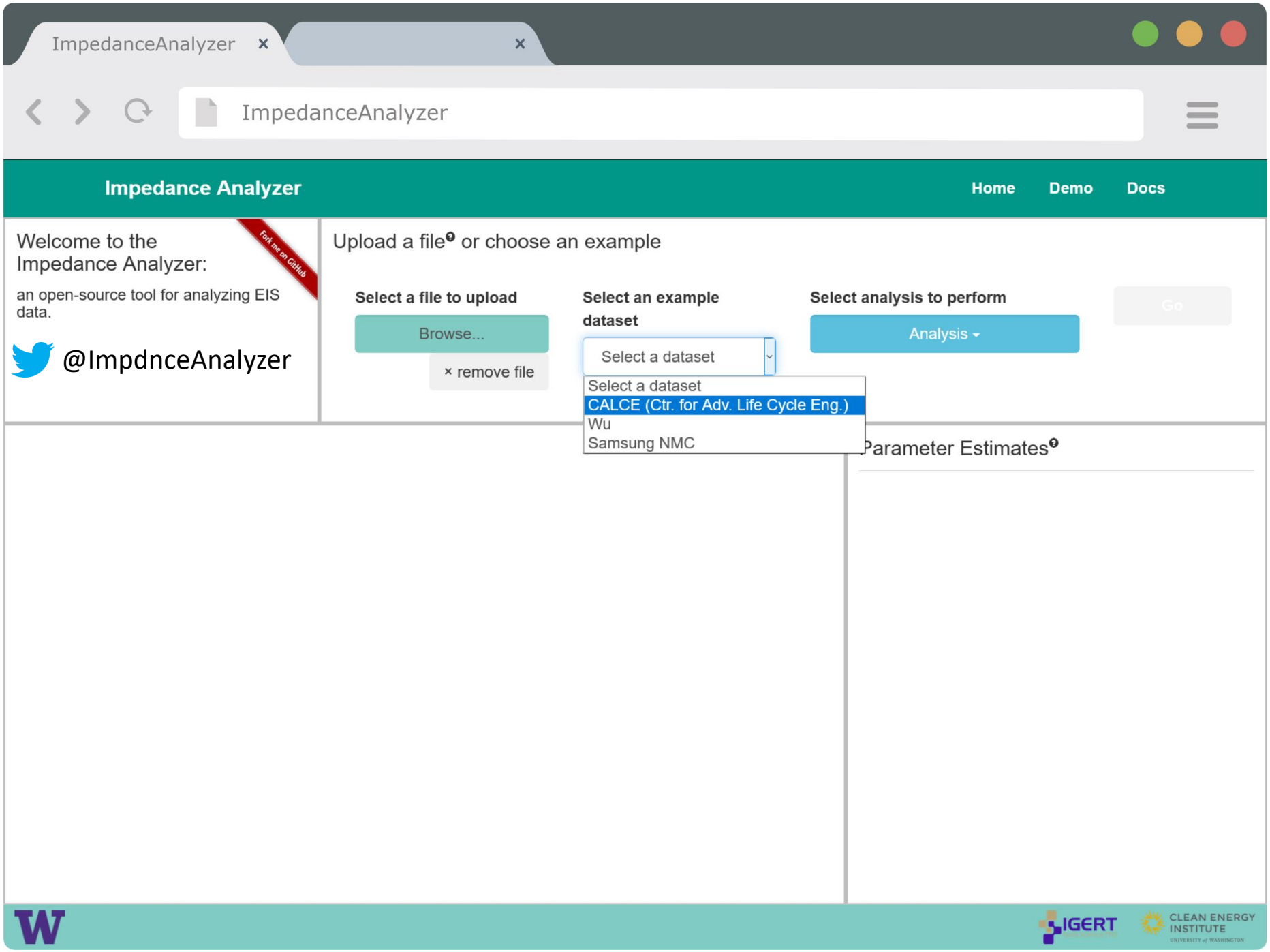
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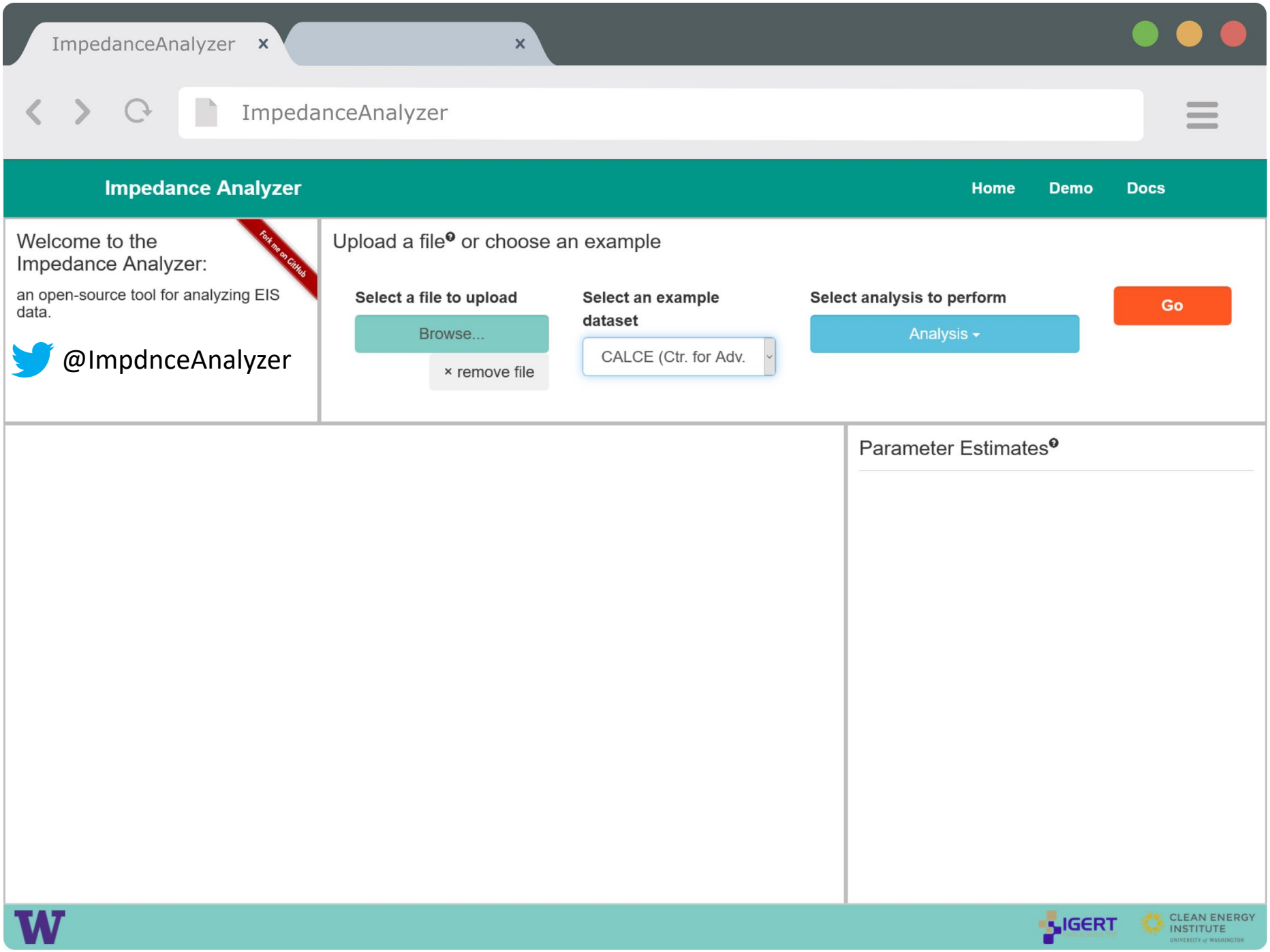
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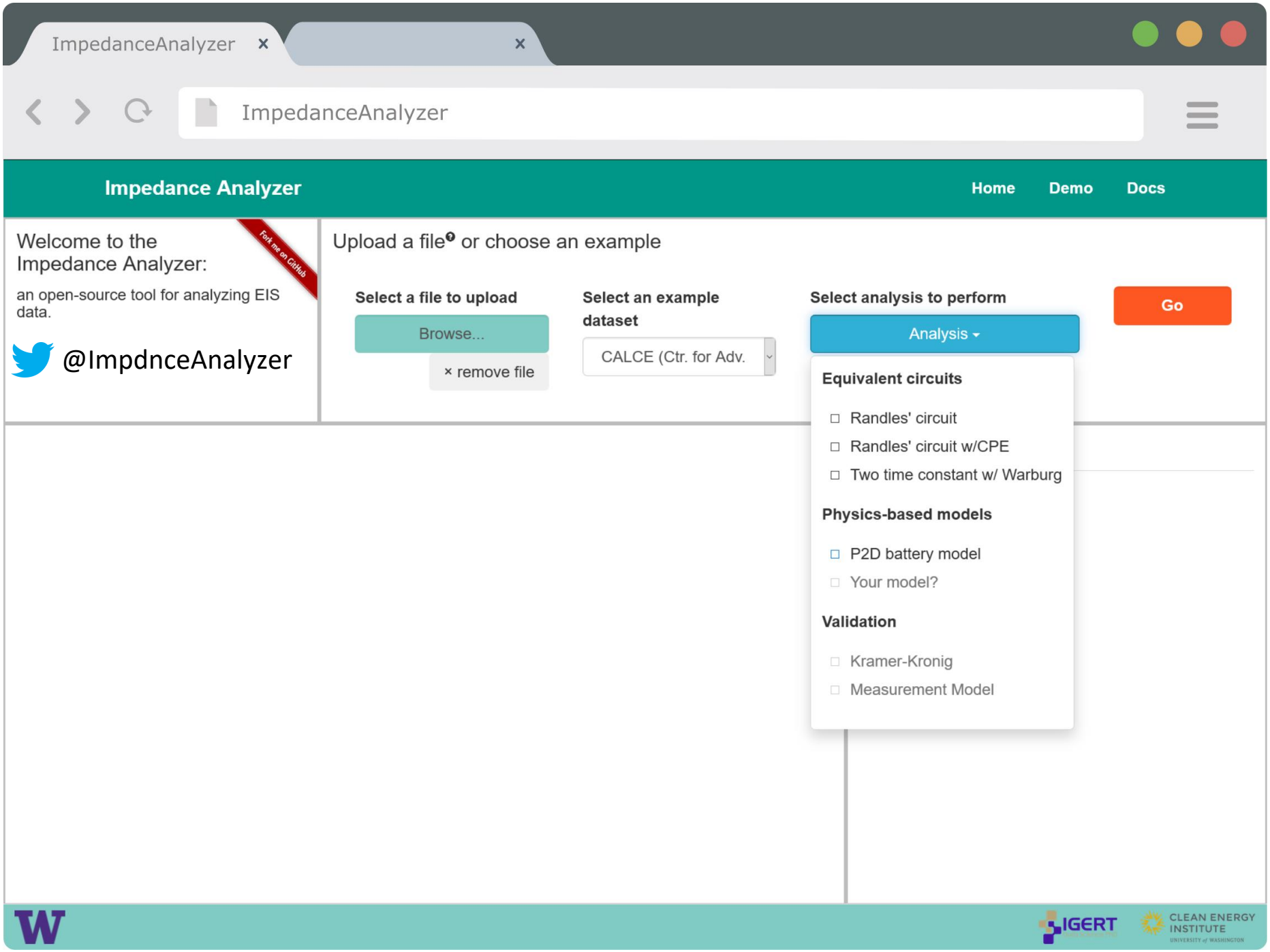
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Randles' circuit
Randles' circuit w/CPE
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P2D battery model
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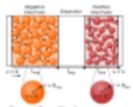
Input options for model fits



Pseudo 2-Dimensional

Select type of fit

- Capacity and Contact Resistance

Capacity (mAh) mAh

Dataset: Initial 40,000 spectra

Finished

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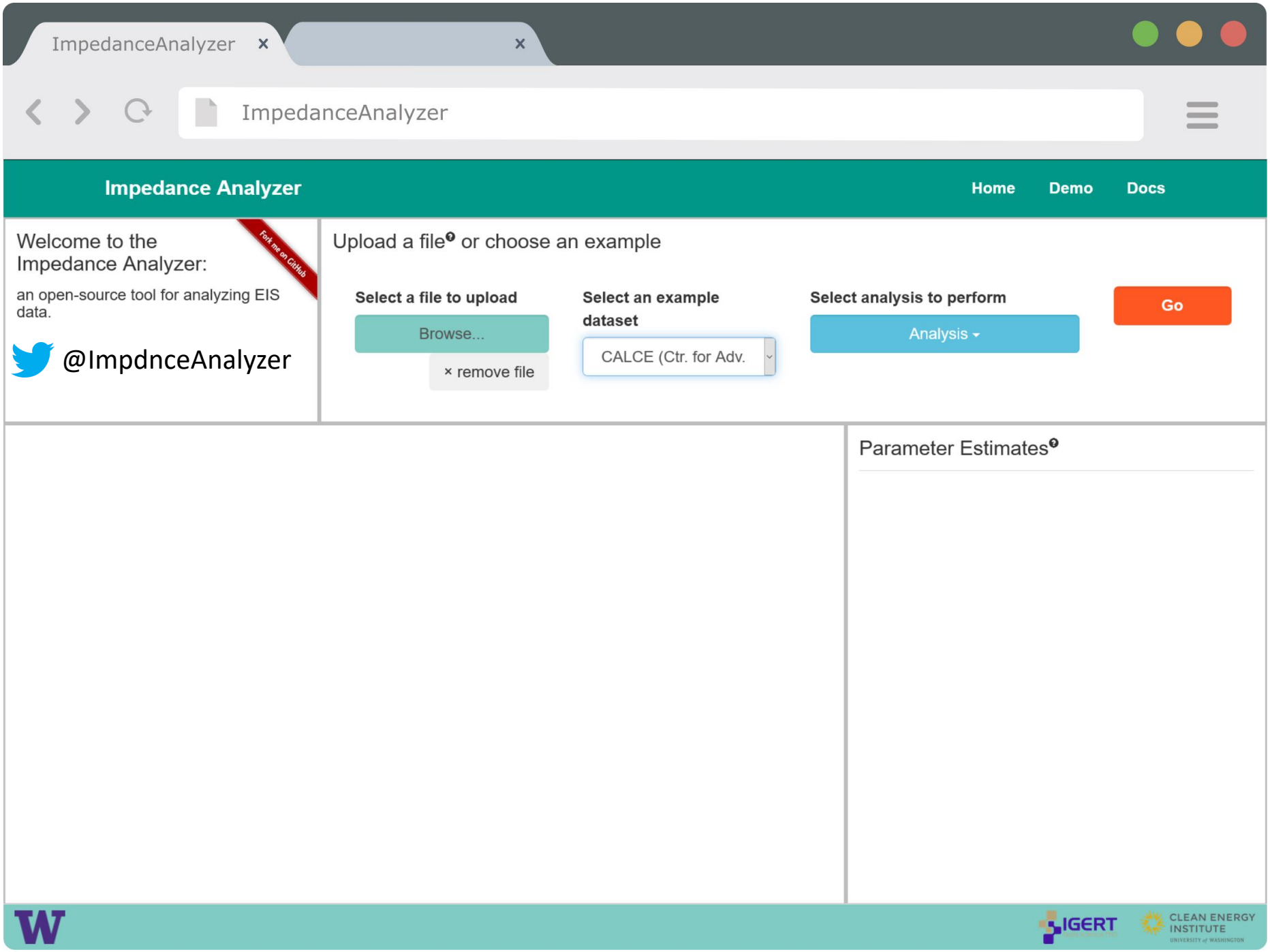
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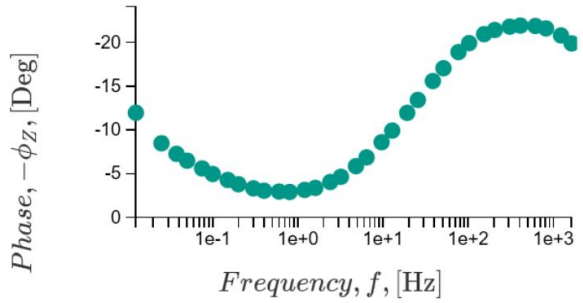

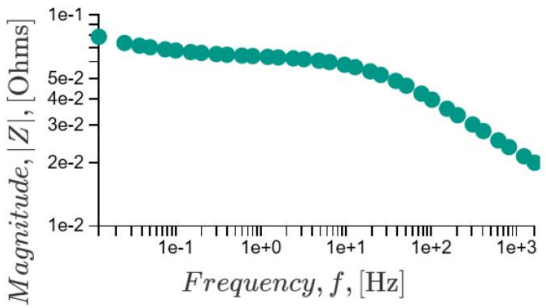

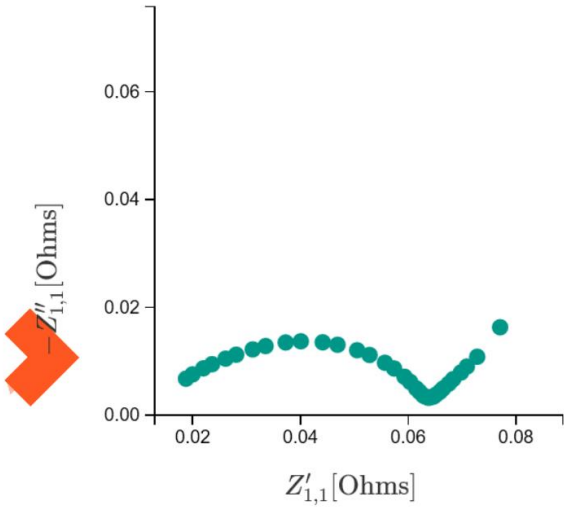

Matching...

Parameter Estimates

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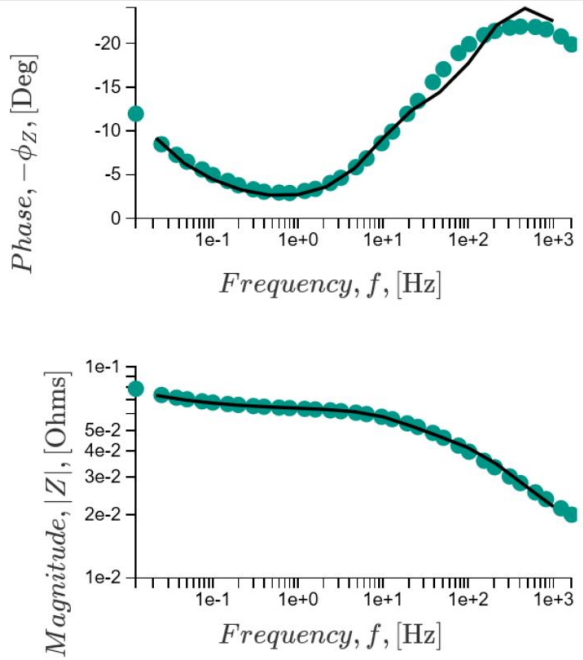

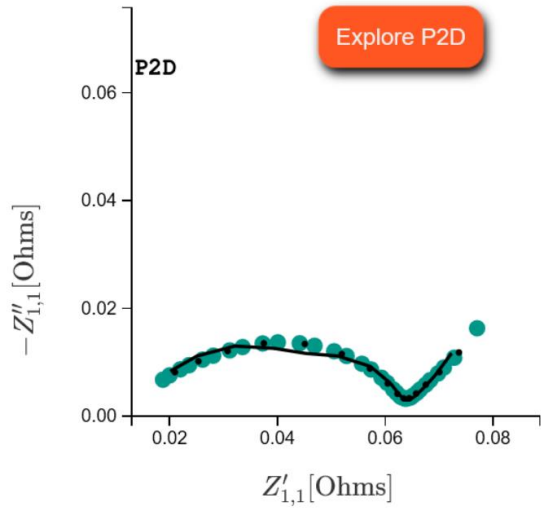

Matching completed in 7 seconds

Parameter Estimates

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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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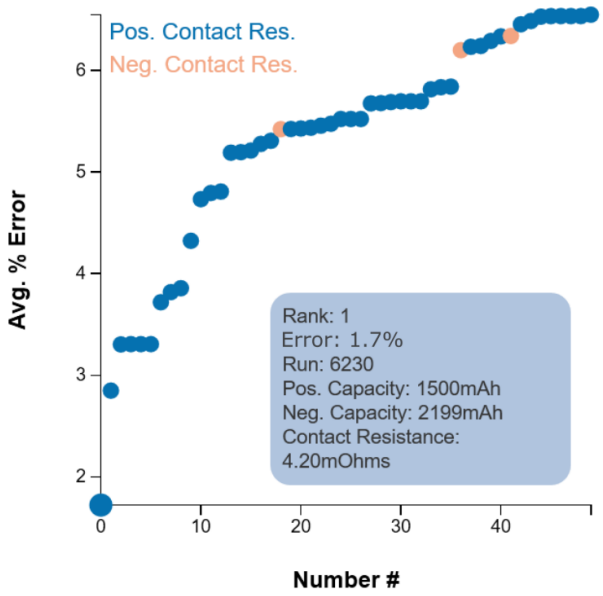
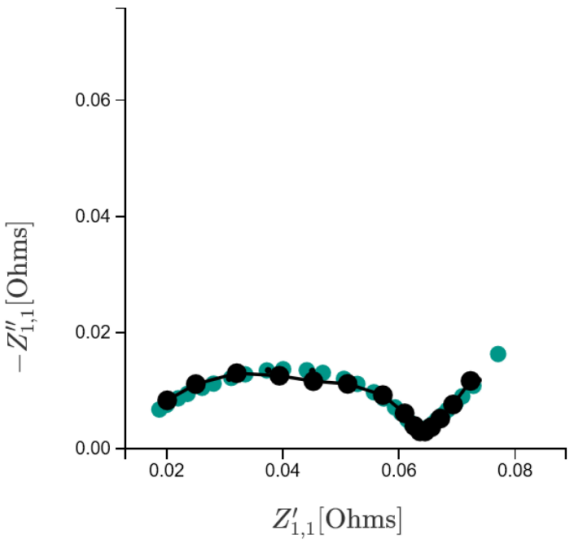
Explore P2D fit





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:

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

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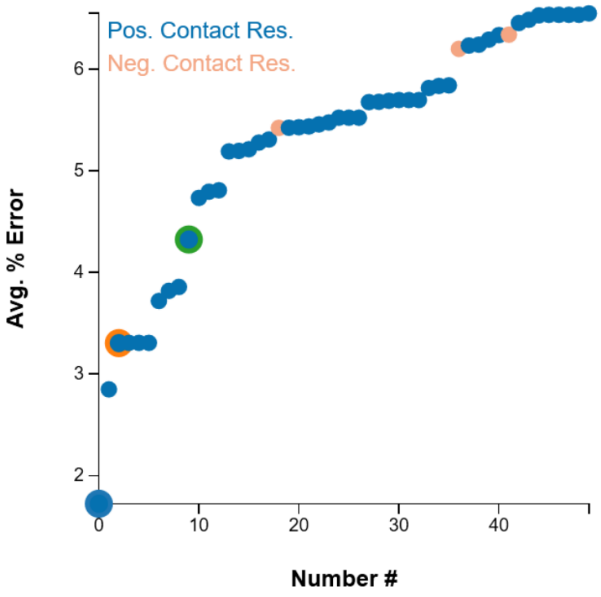
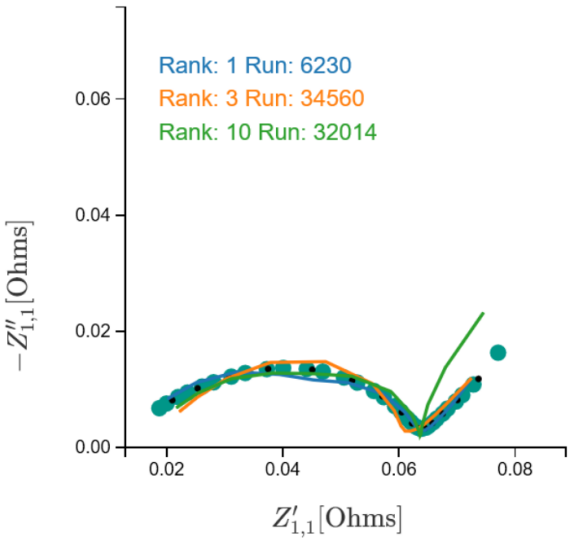
Explore P2D fit

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:

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

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Future work and adding datasets

- The ImpedanceAnalyzer can help bridge the gap between electrochemical modeling and the experimental analysis of EIS spectra
- Open source platform meant for collaboration
- Datasets can be research products and help improve widespread use and impact of models

Looking for a few beta testers (experimental users) and additional datasets: **mmurbach@uw.edu**

For updates and more information…

@ImpdnceAnalyzer

the.impedance.analyzer@gmail.com

Acknowledgements

Prof. Dan Schwartz
Prof. Hanna Hajishirzi

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IGERT Data Science PhD

(slides: mattmurbach.com/slides)