



The ImpedanceAnalyzer:

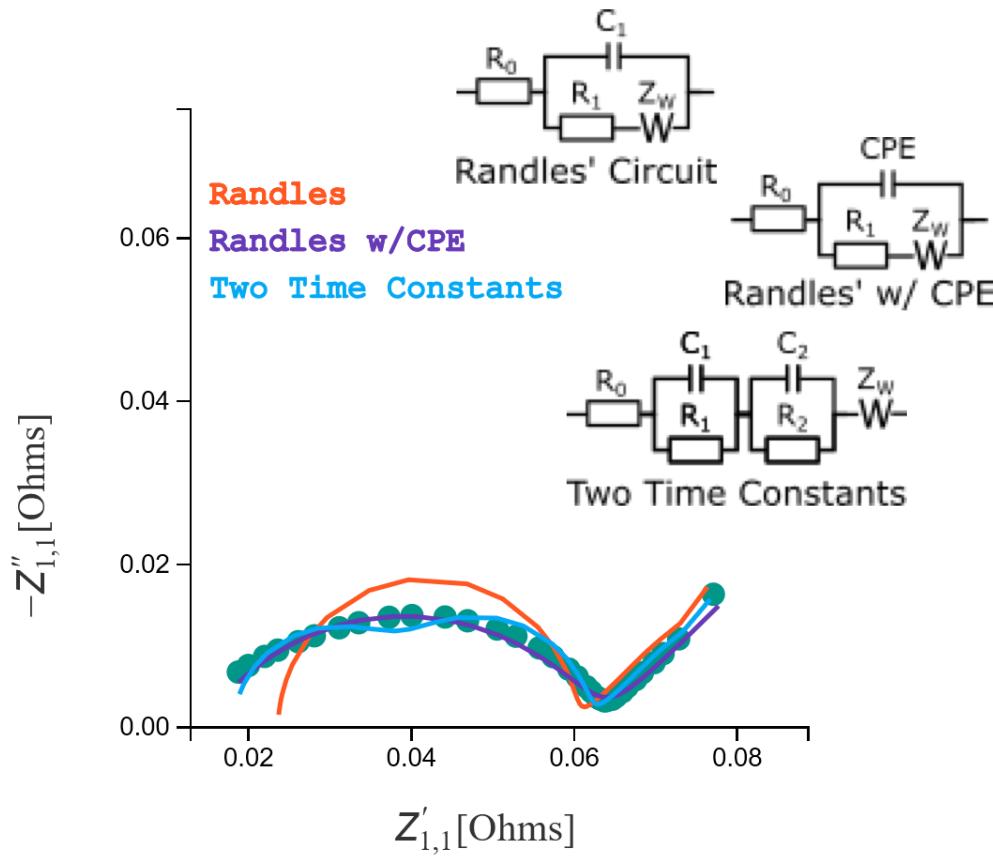
An open-source, web-based tool for sophisticated interrogation of experimental EIS spectra

Matthew D. Murbach, Victor W. Hu, and Daniel T. Schwartz

University of Washington, Seattle
Department of Chemical Engineering
Clean Energy Institute

Tuesday, 3 October 2017
232nd ECS Meeting, National Harbor, MD

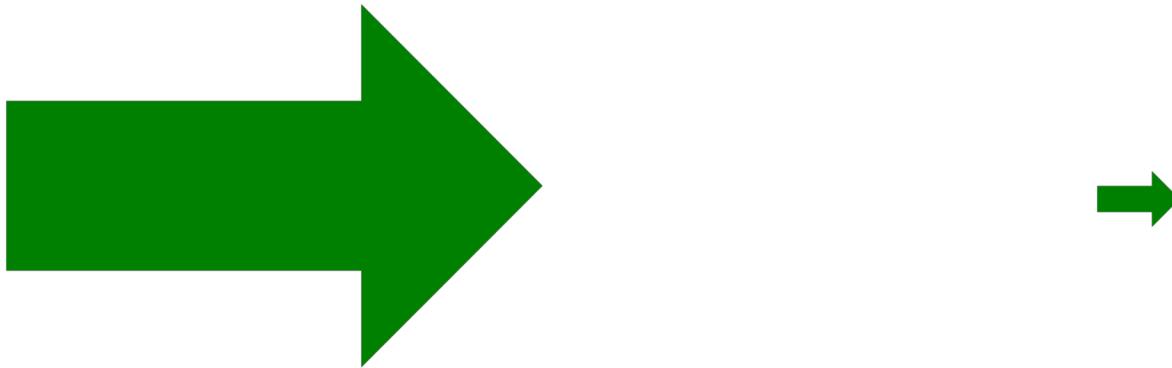
Standard analysis of EIS spectra involves fitting a circuit



Equivalent circuits can capture differences in spectra, but complex circuits can have **tenuous connections to physics**

Fitting physics-based models to EIS data is rare

- 100s of papers using P2D model for battery simulation and design
- Only a handful of models ever applied to impedance analysis
- 3 of top 10 citations in Journal of Electrochemical Society
- Huge loss in translating from modeling to experimental application



- 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 models are hard for experimentalists to use

Solid-Phase Material Balance

$$\text{Real: } \epsilon\omega_1 c_{1,1}^{s''} = \frac{1}{r^2} \frac{\partial}{\partial r} (D_s r^2 \frac{\partial c_{1,1}^{s'}}{\partial r}) \quad [\text{A1.1r}]$$

$$\text{Imaginary: } -\epsilon\omega_1 c_{1,1}^{s'} = \frac{1}{r^2} \frac{\partial}{\partial r} (D_s r^2 \frac{\partial c_{1,1}^{s''}}{\partial r}) \quad [\text{A1.1i}]$$

$$\text{BC at } r = R_p: -D_s \frac{\partial c_{1,1}^{s'}}{\partial r} = j_{f,1,1}$$

$$-D_s \frac{\partial c_{1,1}^{s''}}{\partial r} = j_{f,1,1}$$

$$\text{BC at } r = 0: \frac{\partial c_{1,1}^{s'}}{\partial r} = 0 \quad \frac{\partial c_{1,1}^{s''}}{\partial r} = 0$$

Solution-Phase Material Balance

$$\text{Real: } \frac{\partial}{\partial x} (D_{eff} \frac{\partial c_{1,1}^{s'}}{\partial x}) = \epsilon\omega_1 c_{1,1}'' - a(1 - t_+^0)(j_{f,1,1} + j_{dl,1,1}) \quad [\text{A1.2r}]$$

$$\text{Imaginary: } \frac{\partial}{\partial x} (D_{eff} \frac{\partial c_{1,1}^{s''}}{\partial x}) = -\epsilon\omega_1 c_{1,1}' - a(1 - t_+^0)(j_{f,1,1}'' + j_{dl,1,1}'') \quad [\text{A1.2i}]$$

$$\text{BC at } x = 0 \text{ and } x = l_{neg} + l_{sep} + l_{pos}: \frac{\partial c_{1,1}^{s'}}{\partial x} = 0 \quad \frac{\partial c_{1,1}^{s''}}{\partial x} = 0$$

Faraday's Law

$$\text{Real: } \frac{\partial i_{2,1,1}'}{\partial x} = aF(j_{f,1,1} + j_{dl,1,1}) \quad [\text{A1.3r}]$$

$$\text{Imaginary: } \frac{\partial i_{2,1,1}''}{\partial x} = aF(j_{f,1,1}'' + j_{dl,1,1}'') \quad [\text{A1.3i}]$$

$$\text{BC at } x = 0 \text{ and } x = L: i_{2,1,1}' = 0 \quad i_{2,1,1}'' = 0$$

$$\text{BC at } x = l_{neg} \text{ and } x = l_{neg} + l_{sep}: i_{2,1,1}' = -1 \quad i_{2,1,1}'' = 0$$

Solid-Phase Potential

$$\text{Real: } -\sigma_{eff} \frac{\partial \varphi_{1,1}'}{\partial x} = -1 - i_{2,1,1}' \quad [\text{A1.4r}]$$

$$\text{Imaginary: } -\sigma_{eff} \frac{\partial \varphi_{1,1}''}{\partial x} = -i_{2,1,1}'' \quad [\text{A1.4i}]$$

$$\text{BC at } x = 0 \text{ and } x = L: \sigma_{eff} \frac{\partial \varphi_{1,1}'}{\partial x} = 1$$

$$\frac{\partial \varphi_{1,1}''}{\partial x} = 0$$

$$\text{BC at } x = l_{neg} \text{ and } x = l_{neg} + l_{sep}: \frac{\partial \varphi_{1,1}'}{\partial x} = 0 \quad \frac{\partial \varphi_{1,1}''}{\partial x} = 0$$

Solution-Phase Potential

$$\text{Real: } -\kappa_{eff} \frac{\partial \varphi_{1,1}'}{\partial x} = i_{2,1,1}' - \frac{2\kappa_{eff}RT}{c_0 F} (1 - t_+^0) \frac{\partial c_{1,1}'}{\partial x} \quad [\text{A1.5r}]$$

$$\text{Imaginary: } -\kappa_{eff} \frac{\partial \varphi_{1,1}''}{\partial x} = i_{2,1,1}'' - \frac{2\kappa_{eff}RT}{c_0 F} (1 - t_+^0) \frac{\partial c_{1,1}''}{\partial x} \quad [\text{A1.5i}]$$

$$\text{BC at } x = 0: \varphi_{1,1}' = 0 \quad \varphi_{1,1}'' = 0$$

$$\text{BC at } x = l_{neg} + l_{sep} + l_{pos}: \frac{\partial \varphi_{1,1}'}{\partial x} = 0 \\ \frac{\partial \varphi_{1,1}''}{\partial x} = 0$$

Faradaic Flux

$$\text{Real: } j_{f,1,1}' = \frac{i_0(\alpha_a + \alpha_c)}{RT} \eta_{1,1}' \quad [\text{A1.6r}]$$

$$\text{Imaginary: } j_{f,1,1}'' = \frac{i_0(\alpha_a + \alpha_c)}{RT} \eta_{1,1}'' \quad [\text{A1.6i}]$$

Double-layer Flux

$$\text{Real: } j_{dl,1,1}' = \omega_1 \frac{C_{dl}}{F} (\varphi_{1,1}'' - \varphi_{1,1}') \quad [\text{A1.7r}]$$

$$\text{Imaginary: } j_{dl,1,1}'' = \omega_1 \frac{C_{dl}}{F} (\varphi_{1,1}' - \varphi_{1,1}^s) \quad [\text{A1.7i}]$$

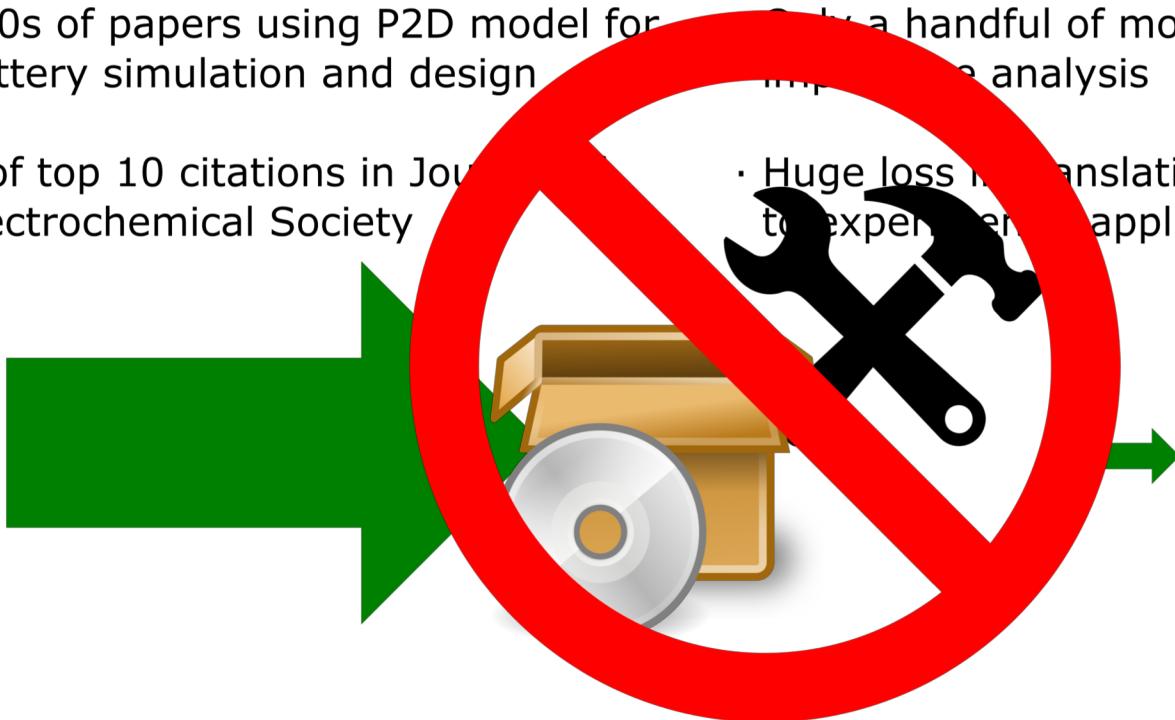
Overpotential

$$\text{Real: } \eta_{1,1}' = \varphi_{1,1}'' - \varphi_{1,1}' - \frac{dU}{dc^s} c_{1,1}^{s'} \quad [\text{A1.8r}]$$

$$\text{Imaginary: } \eta_{1,1}'' = \varphi_{1,1}''' - \varphi_{1,1}'' - \frac{dU}{dc^s} c_{1,1}^{s''} \quad [\text{A1.8i}]$$

We're missing the tools and software to make it easy

- 100s of papers using P2D model for battery simulation and design
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The ImpedanceAnalyzer

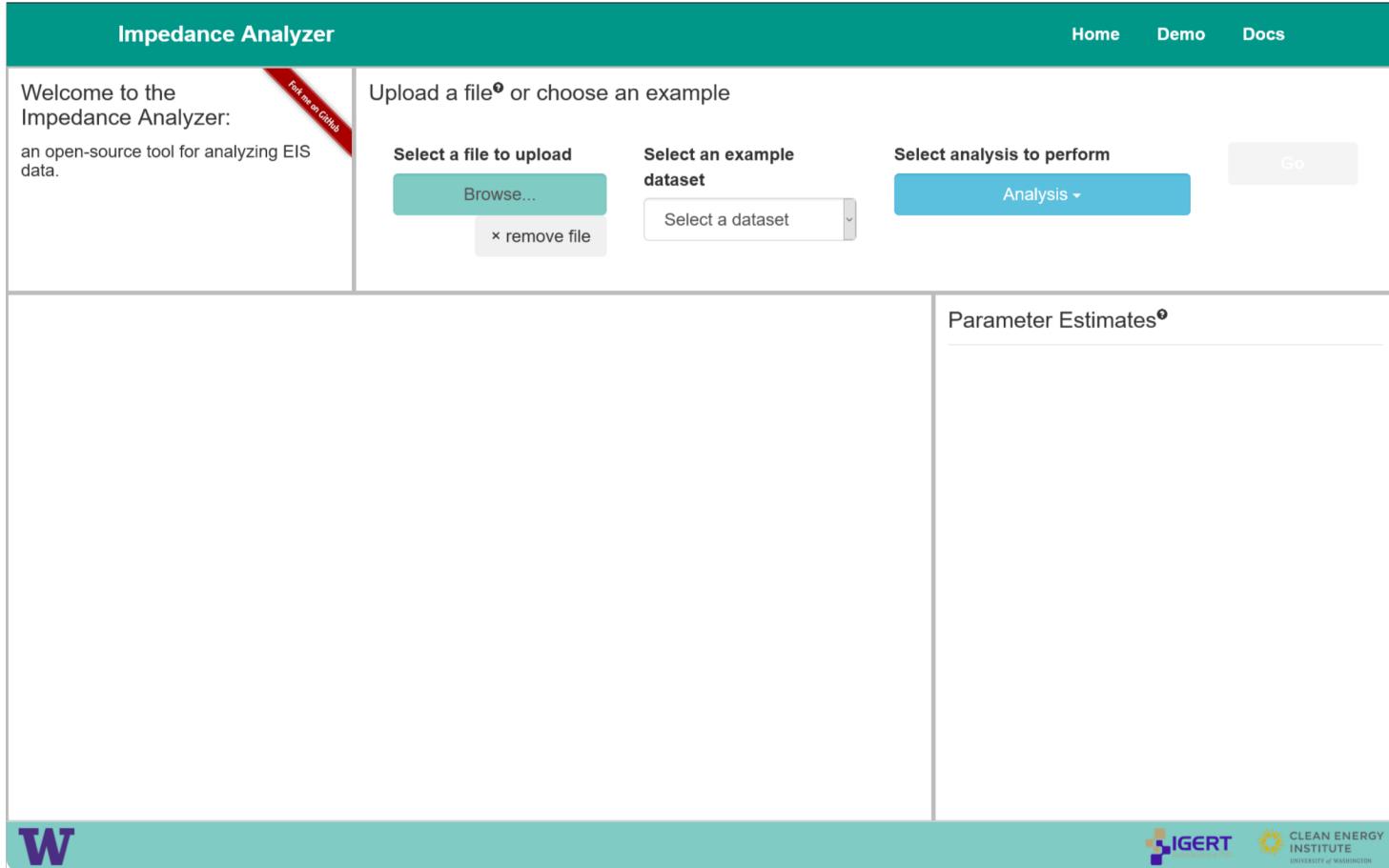
Goal: create a open platform for reproducible and sophisticated analysis of impedance spectra



A Python backend +
JavaScript frontend make
sophisticated analyses
and useful interactive
visualizations possible

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How it works: theimpedanceanalyzer.com



The screenshot shows the homepage of the Impedance Analyzer. At the top, there's a green header bar with the title "Impedance Analyzer" on the left and navigation links "Home", "Demo", and "Docs" on the right. Below the header, the main content area has a white background. On the left, a sidebar contains the text: "Welcome to the Impedance Analyzer: an open-source tool for analyzing EIS data." A red "Fork me on GitHub" button is positioned above this text. To the right of the sidebar, there are three main input fields: "Upload a file" with a "Browse..." button, "Select an example dataset" with a dropdown menu, and "Select analysis to perform" with a dropdown menu set to "Analysis". A "Go" button is located to the right of the analysis dropdown. On the far right, a large section is titled "Parameter Estimates" with a sub-section for "EIS Data". At the bottom of the page, there's a teal footer bar featuring the University of Washington logo ("W") on the left, and logos for IGERT, CLEAN ENERGY INSTITUTE, and UNIVERSITY OF WASHINGTON on the right.

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How it works: uploading data

Upload a file[?] or choose an example

The screenshot shows a user interface for uploading data and performing analysis. At the top, there are three main sections: "Select a file to upload" (with a "Browse..." button and an "x remove file" link), "Select an example dataset" (with a dropdown menu showing "Select a dataset"), and "Select analysis to perform" (with a dropdown menu currently set to "Analysis"). To the right of these is a large orange "Go" button. A detailed view of the "Select analysis to perform" section is shown in a modal window:

- Equivalent circuits**
 - Randles' circuit
 - Randles' circuit w/CPE
 - Two time constant w/ Warburg
- Physics-based models**
 - P2D battery model
 - Your model?
- Validation**
 - Kramer-Kronig
 - Measurement Model

How it works: fitting spectra

Impedance Analyzer

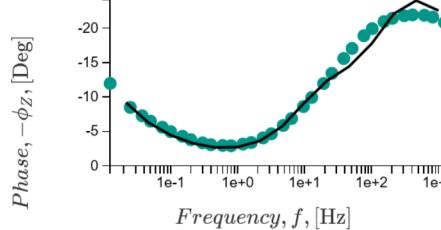
Welcome to the Impedance Analyzer:
an open-source tool for analyzing EIS data.

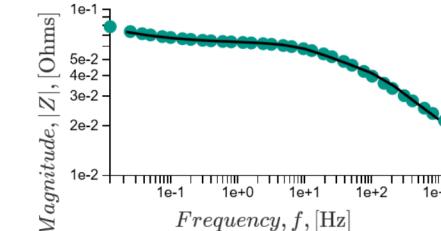
Upload a file^① or choose an example

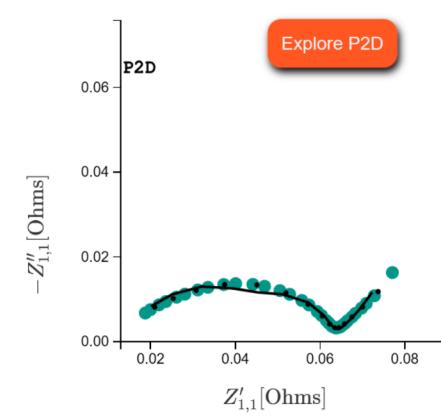
Select a file to upload
[Browse...](#) [x remove file](#)

Select an example dataset
CALCE (Ctr. for Adv.)

Select analysis to perform
Analysis ▾ [Go](#)







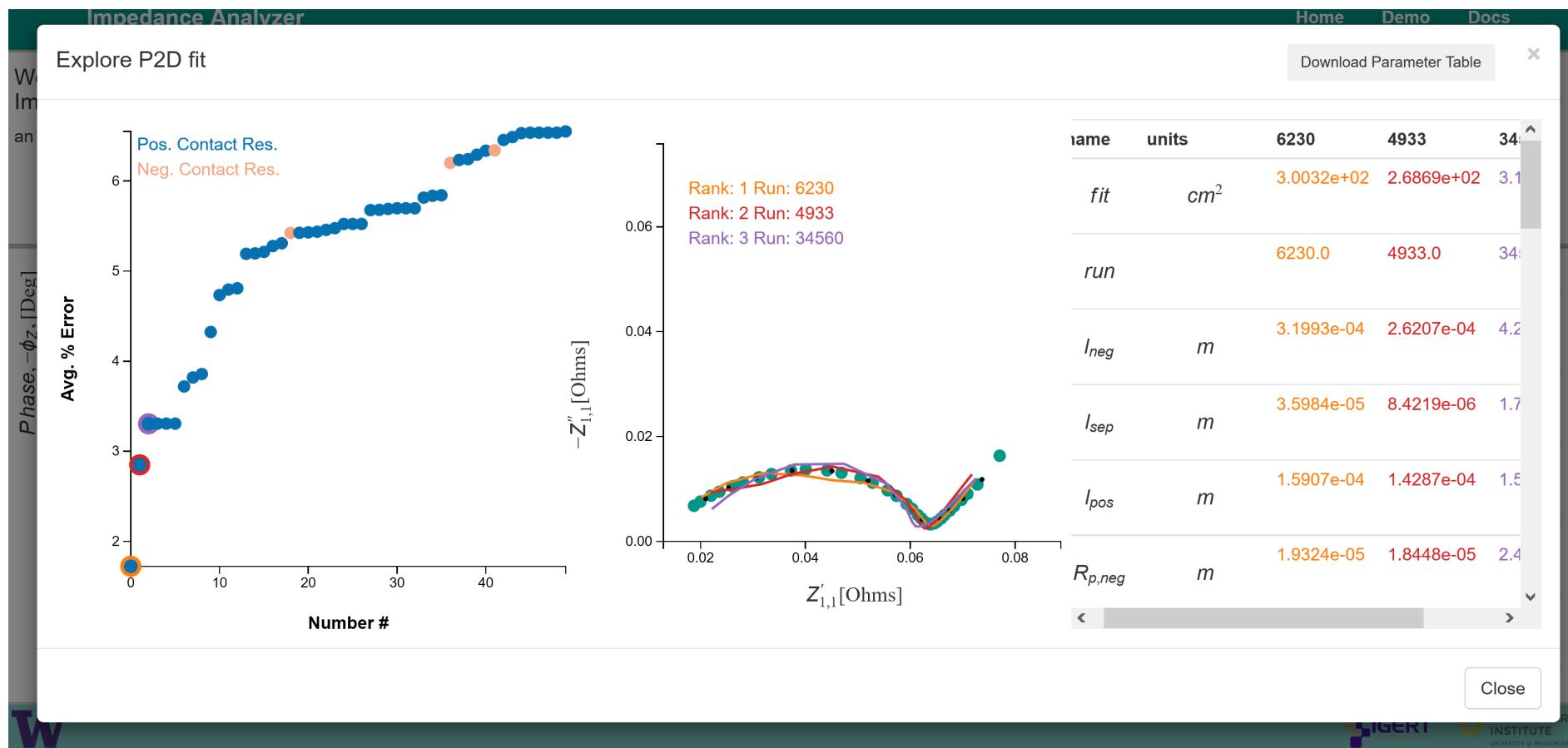
Parameter Estimates^② [Download Results](#)

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

Matching completed in 7 seconds



How it works: interactive visualizations



Difference in parameter estimates

Equivalent circuit methods

Randles	Randles w/CPE	Two Time Constants	P2D	
Parameter	Units	Best Estimate	Error ^①	% Error
R_0	Ohms	0.02360	0.001405	5.954
R_1	Ohms	0.03599	0.001614	4.486
C_1	F	0.06510	0.007915	12.16
W_1	Ohms	0.05633	0.02182	38.73
W_2	Sec	57.47	48.48	84.36

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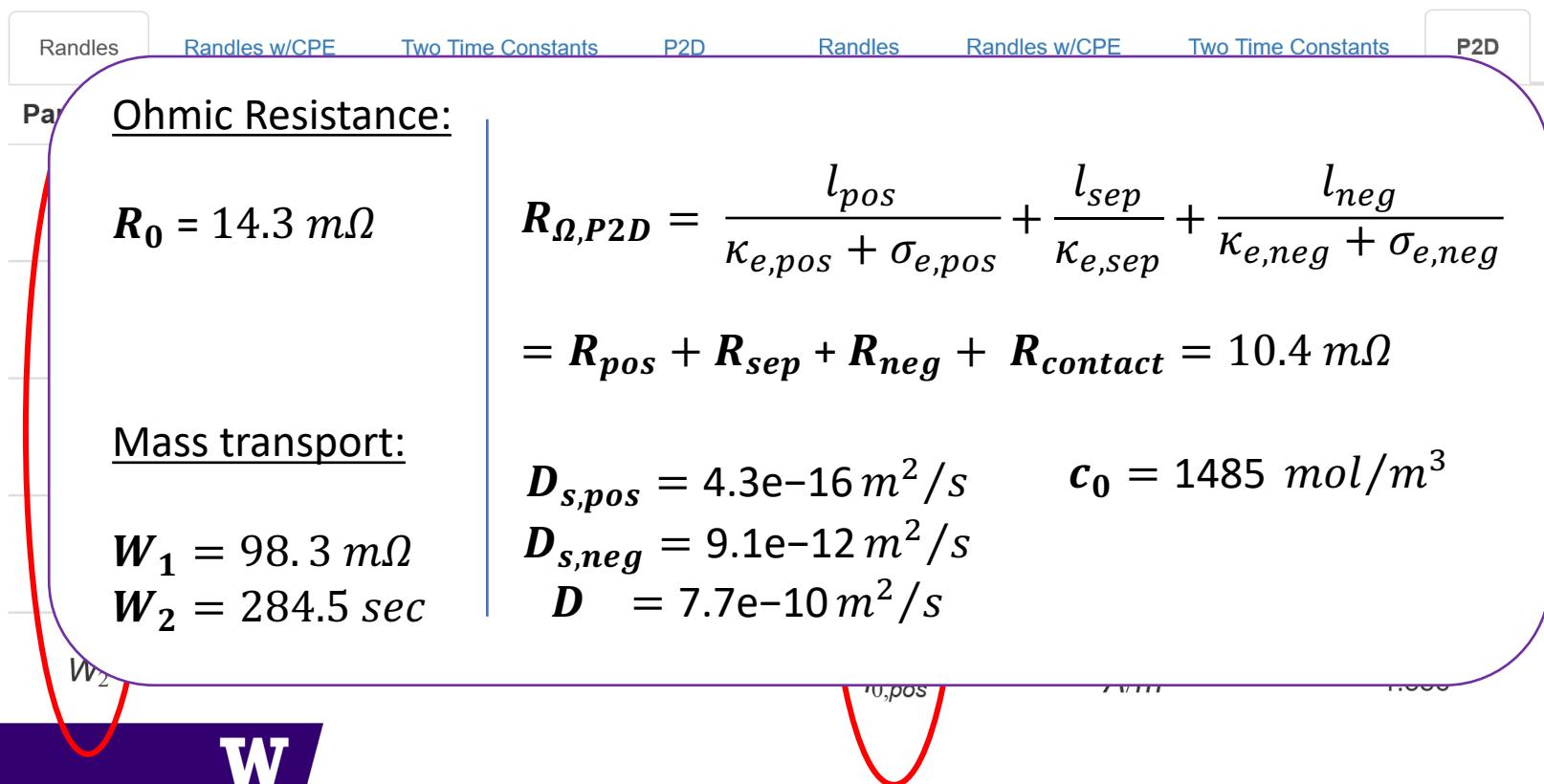
Physics-based model (P2D)

Randles	Randles w/CPE	Two Time Constants	P2D
Parameter	Units	Best Estimate	
D	m^2/s	7.685e-10	
$D_{s,neg}$	m^2/s	9.089e-12	
$D_{s,pos}$	m^2/s	4.337e-16	
$i_{0,neg}$	A/m^2	19.42	
$i_{0,pos}$	A/m^2	1.556	

Difference in parameter estimates

Equivalent circuit methods

Physics-based model (P2D)



Open-source tools give us the opportunity to drive the field forward

- Tools is publicly available (<http://www.theimpedanceanalyzer.com/>)
 - Beta version. Feedback is really helpful!
- Code is on GitHub ([mdmurbach/ImpedanceAnalyzer](https://github.com/mdmurbach/ImpedanceAnalyzer))
 - Use issues to suggest features
 - Pull requests for contributions
 - Star for updates



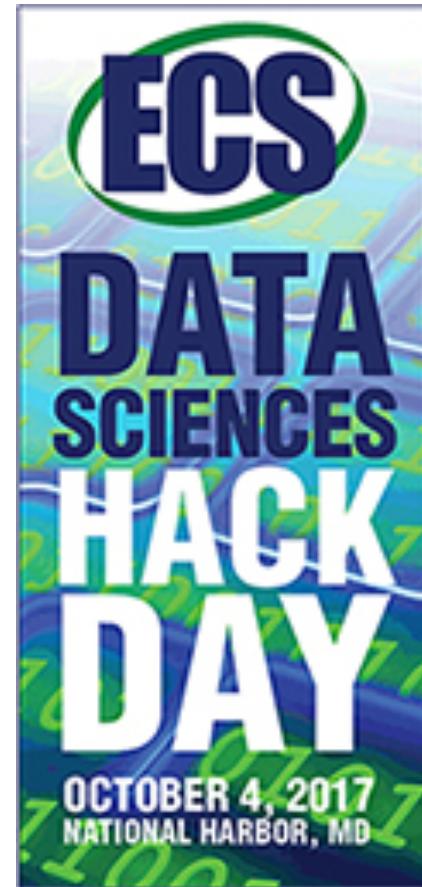
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Thoughts on future features

- Integrate knowledge of known parameters
- Confidence intervals on estimated parameters
- Integrate direct, local optimization of P2D model
- ...
- Add new models/physics?
- Additional UI features?

Next steps

- Building a community of electrochemical + data scientists
- Building a set of community developed tools for electrochemical analysis
- Building a culture valuing open datasets, open software, and impact in addition to manuscripts



Thank you!



slides at mattmurbach.com/slides

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