Mapping Long-Term SOFC Performance versus Initial Microstructure with an Integrated Model and Machine Learning

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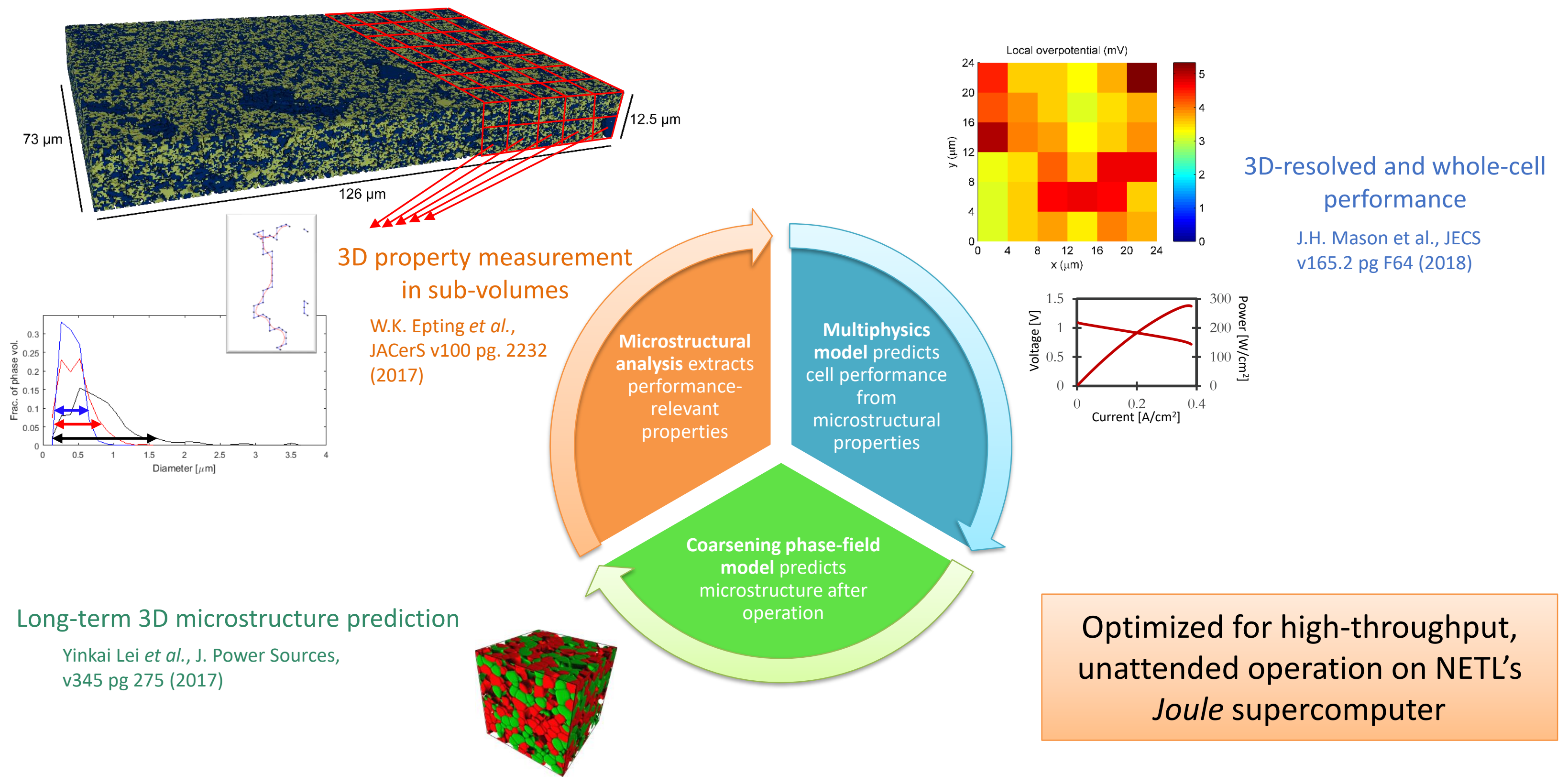
Predicting Long Term SOFC Performance

Long-term performance degradation is a key barrier to SOFC commercialization and the subject of a major DOE technical target (0.2% voltage decay per 1,000 hours). Modelling is key to understanding degradation and predicting the long-term outcome of specific electrode designs. To this end, NETL's SOFC Research Group has developed an integrated degradation model to predict the long-term performance of any electrode.



3D property measurement in sub-volumes

W.K. Epting *et al.*, JACerS v100 pg. 2232 (2017)

Microstructural analysis extracts performance-relevant properties

Multiphysics model predicts cell performance from microstructural properties

Coarsening phase-field model predicts microstructure after operation

3D-resolved and whole-cell performance

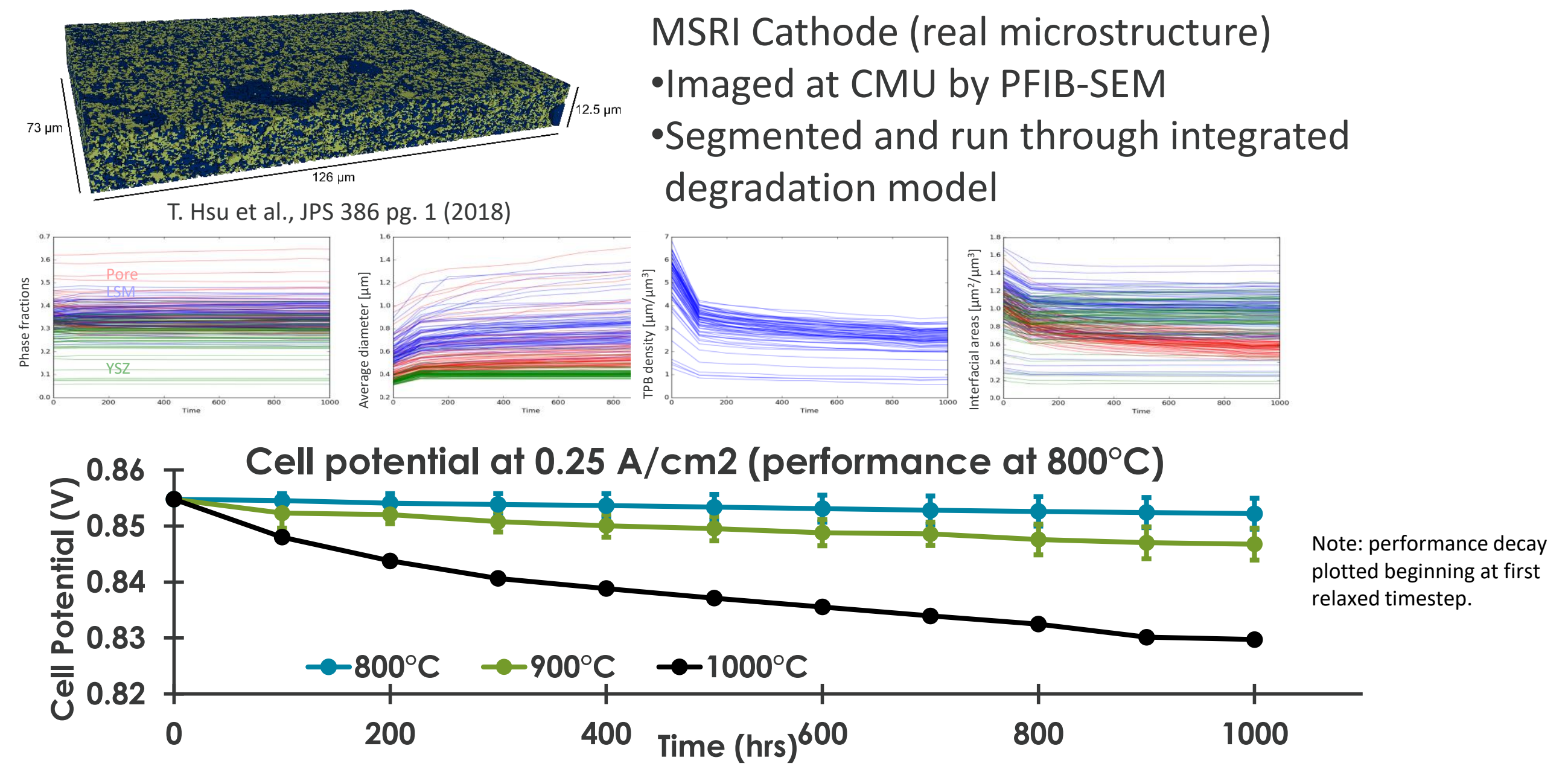
J.H. Mason et al., JECS v165.2 pg F64 (2018)

Long-term 3D microstructure prediction

Yinkai Lei *et al.*, J. Power Sources, v345 pg 275 (2017)

Optimized for high-throughput, unattended operation on NETL's *Joule* supercomputer

Real Electrode Microstructures



T. Hsu et al., JPS 386 pg. 1 (2018)

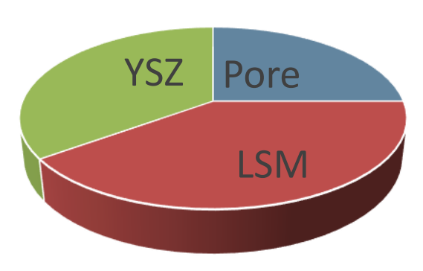
MSRI Cathode (real microstructure)
- Imaged at CMU by PFIB-SEM
- Segmented and run through integrated degradation model

Note: performance decay plotted beginning at first relaxed timestep.

Prediction on real cells is valuable feedback to cell manufacturers. Recommendations for how to improve requires mapping out relationship between microstructure and performance.

Initial Microstructure Defined by 11 Independent Parameters

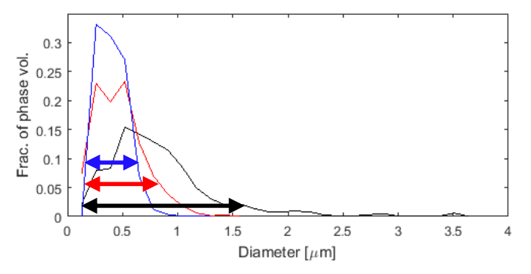
2 independent phase fractions



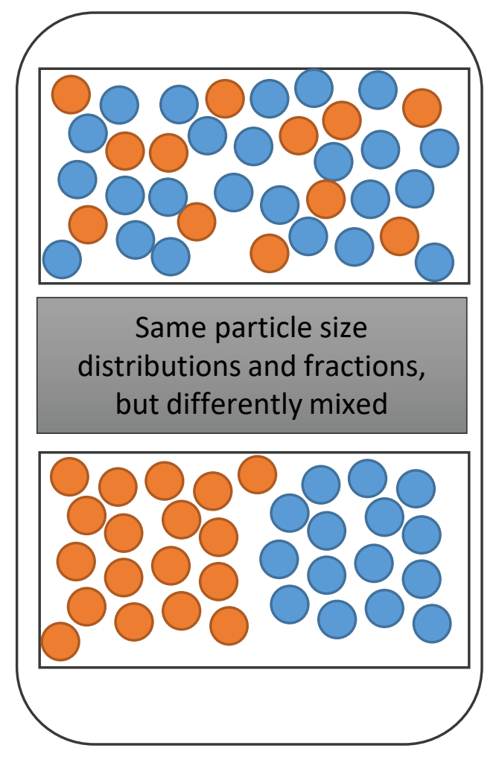
3[rd] fraction set by balancing to 100%

3 average particle/pore sizes

3 particle/pore polydispersity (breadth of distribution)

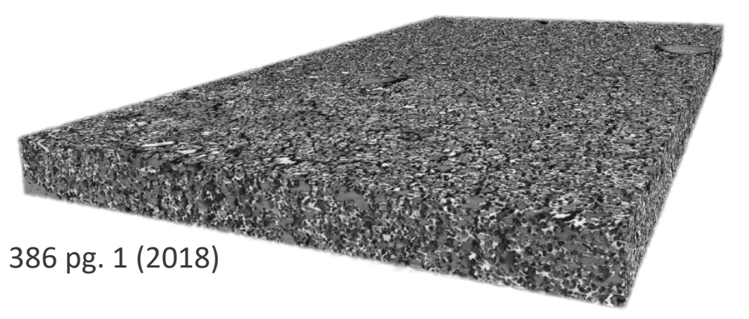


3 phases' heterogeneity or "well-mixedness"



Same particle size distributions and fractions, but differently mixed

Combinations of parameters in 11-dimensional space rapidly approach tens of thousands of electrodes to explore – not feasible when experimental characterization takes days.

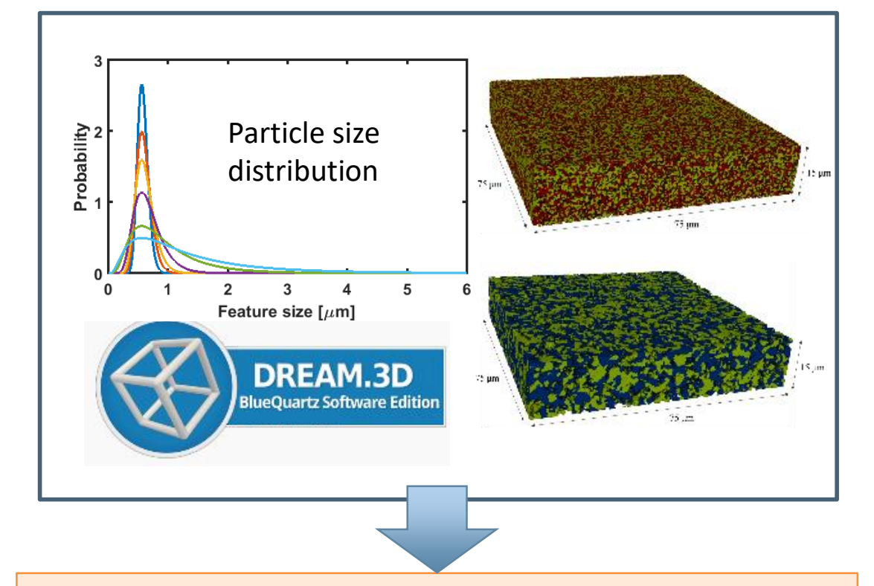


T. Hsu et al., JPS 386 pg. 1 (2018)

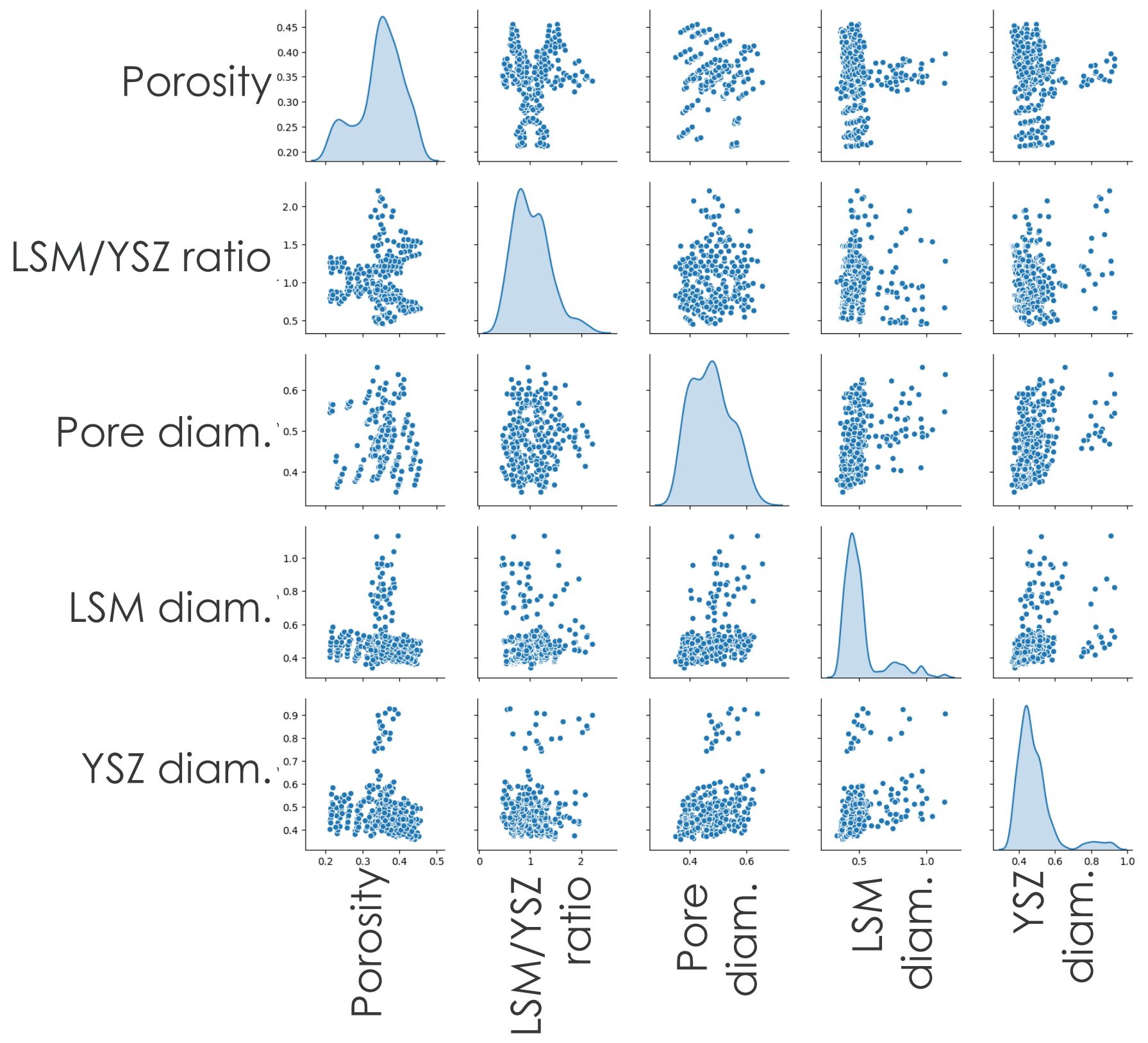
Big Data Approach

Exploring 11D Parameter Space with Simulated Electrodes

Generating synthetic microstructures using DREAM.3D allows deliberate exploration of 11-dimensional parameter space



Bank of 45,000 unique electrodes successfully generated on NETL's *Joule* supercomputer

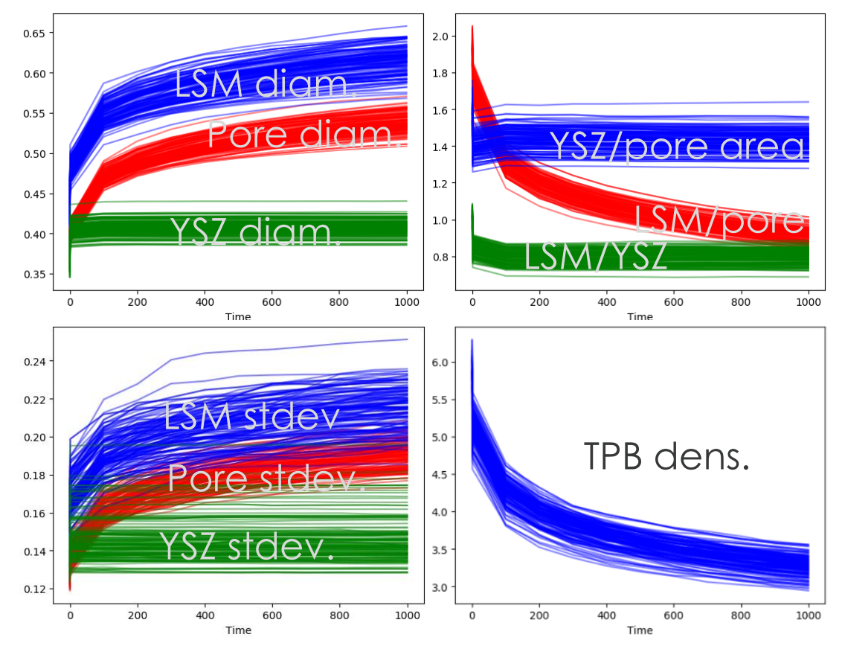


Sub-set of 600 electrodes run through degradation model so far (not all parameters shown)

Evaluating Long-Term Performance

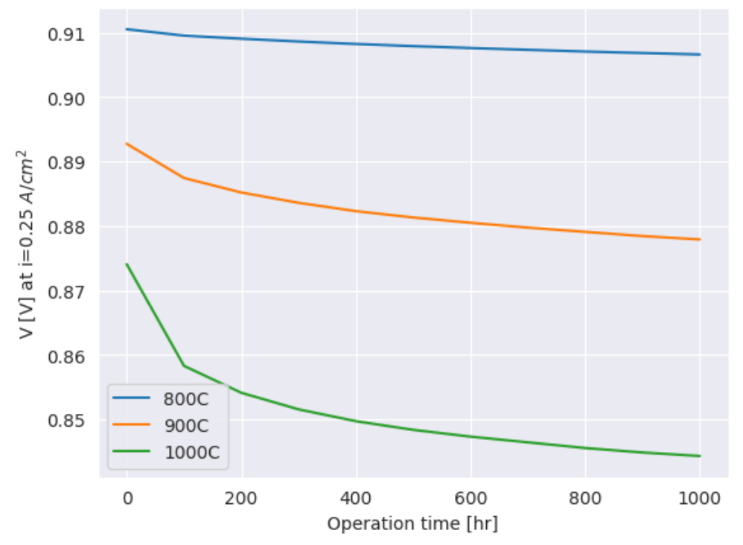
Sample output of one electrode

Microstructural properties over time



At every time step:
- Polarization curves
- Overpotentials
- Spatially resolved current density

Voltage decay over time at 0.25 A/cm²



With hundreds or thousands of electrodes analyzed, it becomes helpful to condense results into a single **figure-of-merit**

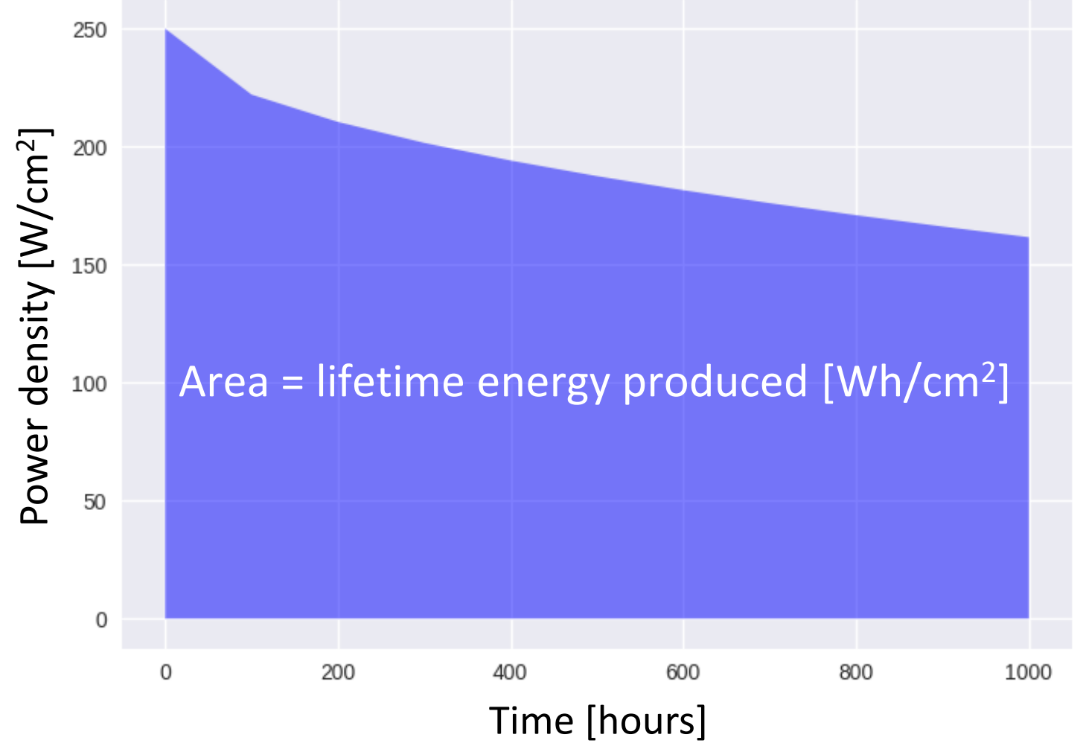
Choose an operational current density (e.g. 0.4 A/cm²)

Energy produced in 1,000 hrs

Captures initial performance as well as decay. **Also a proxy for $/kWh**, a key metric for industry.

ΔV_{cell} from 0 to 1,000 hrs

Voltage decay is important but misses whether electrode was a poor performer to begin with

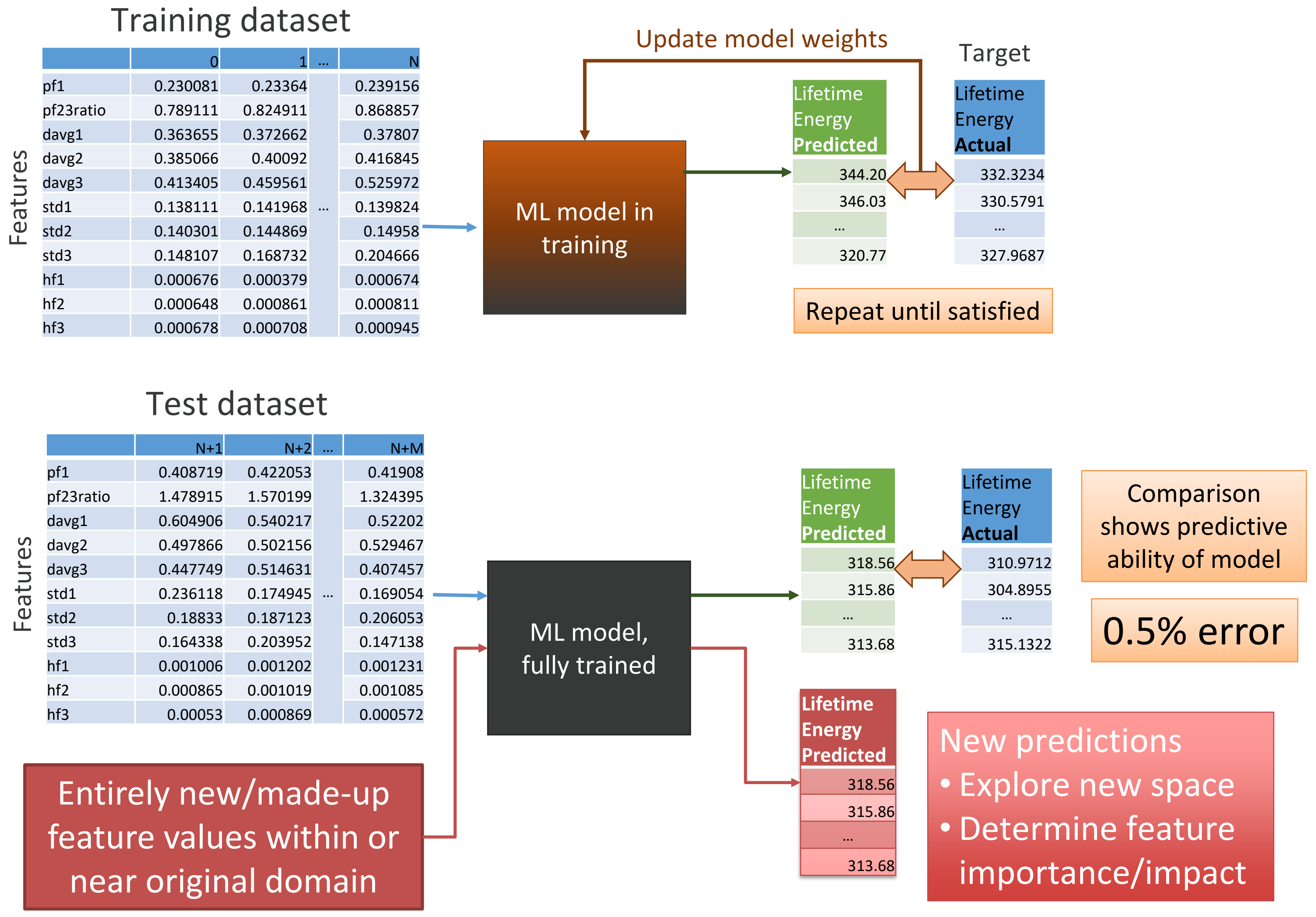


With this choice of figure of merit, we can now map the 11 independent input parameters, or "features," to this 1 outcome value.

Analyzing lifetime energy produced versus one or two features at a time is possible manually, but interrelationships between features makes higher-dimensional analysis difficult. We turn to **machine learning** to better understand the growing bank of high-dimensional results.

Machine Learning Analysis

A neural network model allows us to more deeply examine the relationship between the 11D input space and the outcome, including predicting unexplored portions of space.



Training dataset

	0	1	…	N
pf1	0.230081	0.23364		0.239156
pf23ratio	0.789111	0.824911		0.868857
davg1	0.363655	0.372662		0.37807
davg2	0.385066	0.40092		0.416845
davg3	0.413405	0.459561		0.525972
std1	0.138111	0.141968	…	0.139824
std2	0.140301	0.144869		0.14958
std3	0.148107	0.168732		0.204666
hf1	0.000676	0.000379		0.000674
hf2	0.000648	0.000861		0.000811
hf3	0.000678	0.000708		0.000945

Lifetime Energy **Predicted**	Lifetime Energy **Actual**
344.20	332.3234
346.03	330.5791
…	…
320.77	327.9687

Repeat until satisfied

Test dataset

	N+1	N+2	…	N+M
pf1	0.408719	0.422053		0.41908
pf23ratio	1.478915	1.570199		1.324395
davg1	0.604906	0.540217		0.52202
davg2	0.497866	0.502156		0.529467
davg3	0.447749	0.514631		0.407457
std1	0.236118	0.174945	…	0.169054
std2	0.18833	0.187123		0.206053
std3	0.164338	0.203952		0.147138
hf1	0.001006	0.001202		0.001231
hf2	0.000865	0.001019		0.001085
hf3	0.00053	0.000869		0.000572

Lifetime Energy **Predicted**	Lifetime Energy **Actual**
318.56	310.9712
315.86	304.8955
…	…
313.68	315.1322

Comparison shows predictive ability of model

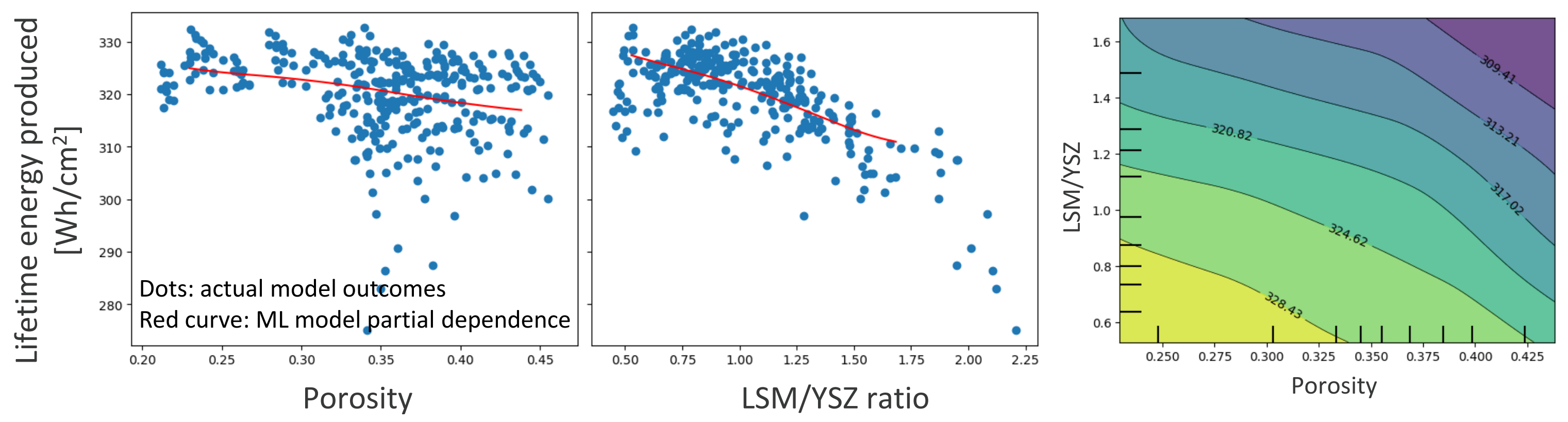
0.5% error

Entirely new/made-up feature values within or near original domain

Lifetime Energy Predicted
318.56
315.86
…
313.68

New predictions
- Explore new space
- Determine feature importance/impact

The trained and validated model allows us to examine the relationship between the model's outcome (lifetime energy produced) and various input parameters (or "features"), for example by mapping the partial dependence of the outcome as one parameter is parametrically varied and others are stochastically varied.

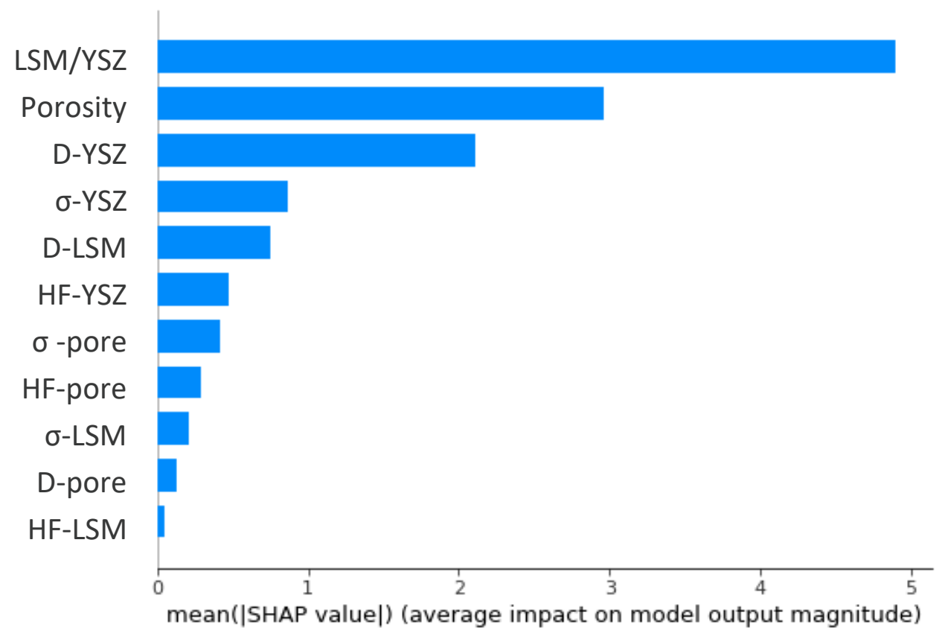


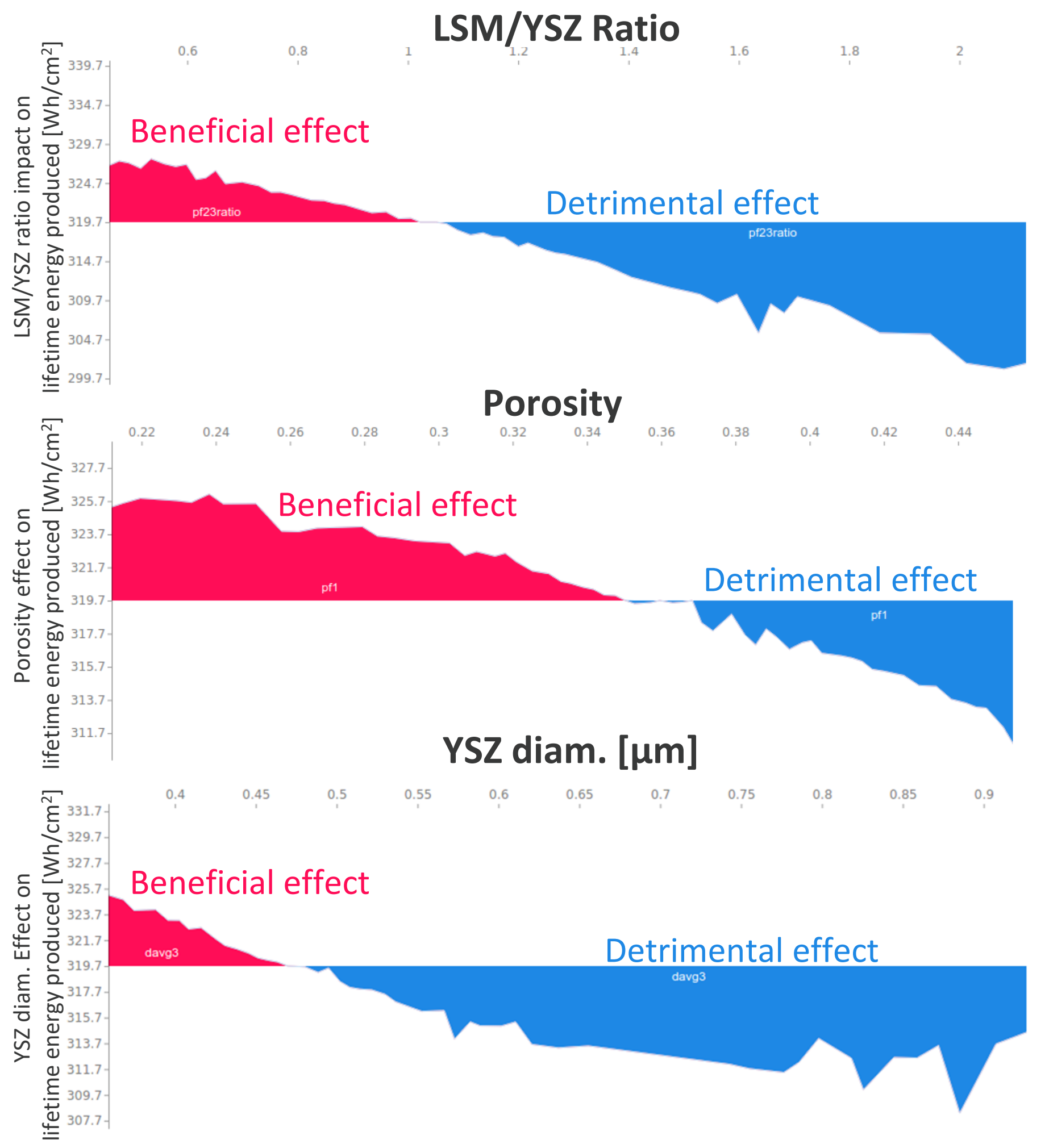
SHAP Values & Feature Importance

SHAP analysis* determines the relative impact on the ML model's predicted outcome of each input/feature versus its mean value, for all cases, allowing the ranking of features by overall importance and the mapping of their impact across parameter space.

* S. M. Lundberg, S-I. Lee. *A Unified Approach to Interpreting Model Predictions.* NIPS 2017.

Feature Importance Rankings





Top-ranking features are recommended for further study.

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