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.

**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.

**Real Electrode Microstructures**

Microstructural properties over time

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.

**Big Data Approach**

Exploring 11D Parameter Space with Simulated Electrodes

Generating synthetic microstructures using DREAM3D allows deliberate exploration of 11-dimensional parameter space.

**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.


**Initial Microstructure Defined by 11 Independent Parameters**

2 independent phase fractions
3 average particle/pore sizes
3 particle/pore polydispersity (breadth of distribution)
3 phases’ heterogeneity or “well-mixedness”

**Evaluating Long-Term Performance**

**Sample output of one electrode**

Microstructural properties over time:
At every time step:
• Polarization curves
• Overpotentials
• Spatially resolved current density

Choose an operational current density (e.g. 0.8 A/cm²)

4Vₘₐₓ 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.

Analysing 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.

**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.

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

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

**Training dataset**

**Test dataset**

**Update model weights**

**Target**

**Comparison shows predictive ability of model**

**New predictions**

• Explore new space
• Determine feature importance/impact

**Energy produced in 1,000 hrs**

Captures initial performance as well as decay. Also a proxy for $5/kWh, a key metric for industry.

**4Vₘₐₓ from 0 to 1,000 hrs**

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**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.


**Feature Importance Rankings**

Top-ranking features are recommended for further study.