**Bayesian Calibration of Models of SOFC Electrode Materials**

Giuseppe F. Brunello, Grigorios Panagakos, Jian Liu, Tobias M. Hunter, Harry O. Finklea, and David S. Mebane.

US Department of Energy, National Energy Technology Laboratory, Pittsburgh, PA / Morgantown, WV; Vienna University of Technology Institute of Chemical Technologies and Analytics Research Division, Vienna, Austria; West Virginia University - Department of Mechanical and Aerospace Engineering, West Virginia University, Morgantown, WV

**Introduction**

Bayesian Theorem is used to update the prior probability of a model’s parameters from experimental evidence to obtain the posterior probability. This is typically done using Markov Chain Monte Carlo since integrating the $P(Z)$ term above is usually, intractable.

To use Bayesian Calibration a Likelihood function is required. This is a statistical model of the process.

**Likelihood function**

$P(Z) = \frac{\prod_{i} f(p_i)}{\int \prod_{i} f(p_i) dp}$

**Experimental Data**

As a result of the Bayesian Calibration, coverage of the experimental data was obtained. Note that there are 200 superimposed line in the figures above.

**Results**

Most of the current is from the TPR reaction; however, as the temperature increases, the fraction of the total current decreases.

**On Going**

The incorporation current vs. distance from the LSM-YSZ interface shows a rapidly decreasing flow of adsorbed ions to LSM vacancies.

**Posterior distribution of the TPR reaction’s activation energy and pre-exponential factor**

Posterior distribution of the Incorporation reaction’s activation energy and pre-exponential factor

Posterior distribution of the Adsorption reaction’s activation energy and pre-exponential factor

We are currently investigating a thin film system at different temperatures and pressure using a modified version of the porous model. Currently, the simulations have not reached equilibrium and the pressure dependence is not yet correct.

**Acknowledgement:** This project was supported in part by an appointment to the Internship Research Participation Program at the National Energy Technology Laboratory, U.S. Department of Energy, administered by the Oak Ridge Institute for Science and Education.