Sequential Monte Carlo Bayesian Calibration of Thin Film Solid Oxide Fuel Cells

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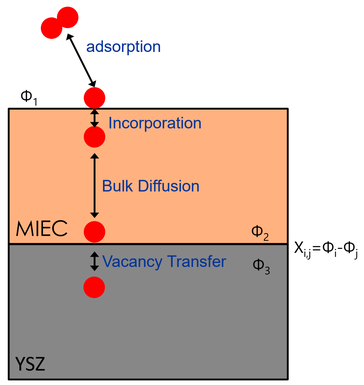
Introduction – Thin Film Model

By using Bayesian calibration to obtain the uncertainty of our parameters, the goal of this study is to identify which material properties change from one sample to the next, and whether a resultant difference is statistically important.

Previously we had developed a porous model of the LSM-YSZ Solid Oxide Fuel Cell (SOFC) system. Therefore we have developed the following Thin Film model by turning off the surface diffusion and triple phase reaction.



Dissociative adsorption:

$$\frac{1}{2}\,O_2(g) + Mn_B^x + V_{ad}^x \longleftrightarrow O'_{ad} + Mn_B^{\cdot}$$

Incorporation:

$$O'_{ad} + V_O^{\cdot\cdot} + Mn_B^x \longleftrightarrow O_O^x + Mn_B^{\cdot} + V_{ad}^x$$

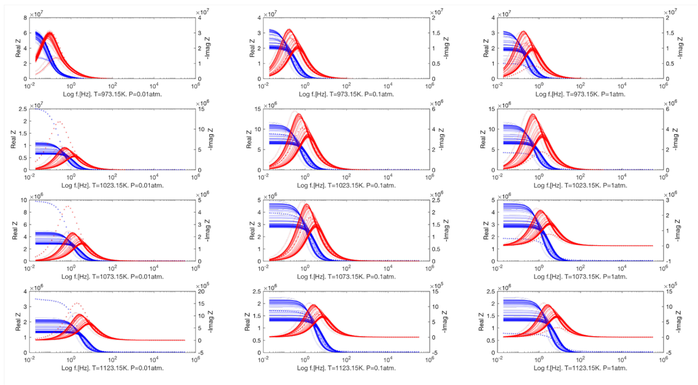
Vacancy Transfer:

$$O_O^x + V_{O,YSZ}^{\cdot\cdot} \longleftrightarrow O_{O,YSZ}^x + V_O^{\cdot\cdot}$$

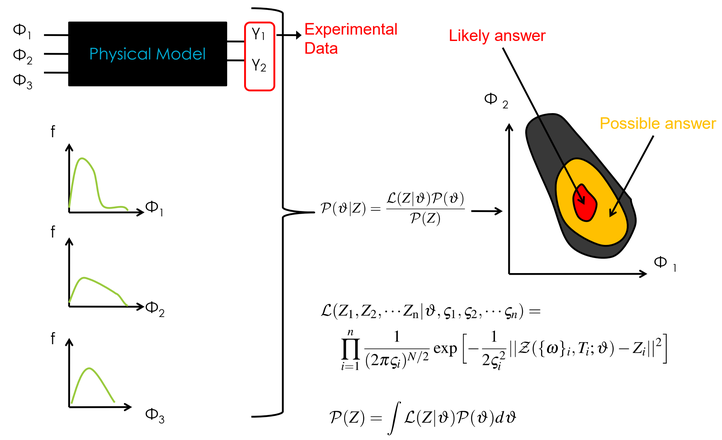
Schottky:

$$nil \longleftrightarrow 3\,V_O^{\cdot\cdot} + V_{La}''' + V_{Mn}'''$$

Although the model is similar to the one successfully calibrated in the porous study, the calibrations of the Thin Film were not as successful:

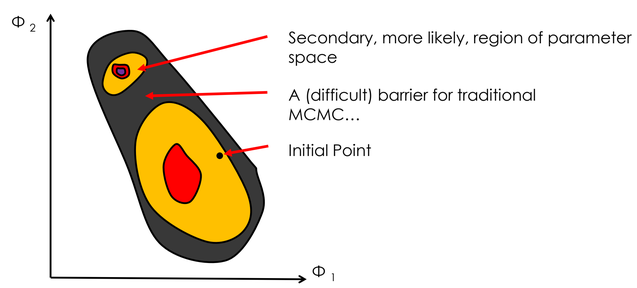


Sequential Monte Carlo



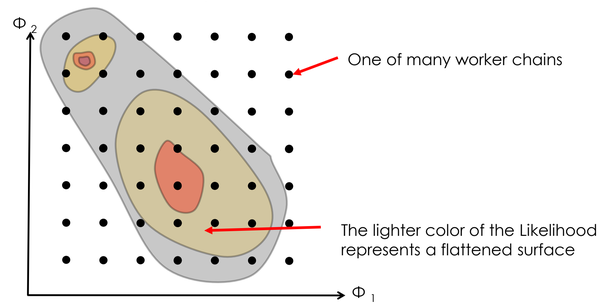
Bayes' Theorem is used to update the prior probability of a model's parameters from experimental evidence to obtain the posterior probability. Typically this is done by Markov Chain Monte Carlo integration (MCMC). But this has two major limitations:

- Cannot be parallelized easily
- Cannot easily overcome barrier to explore all of parameter space



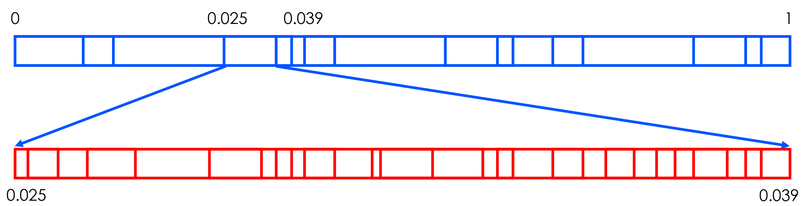
This illustrates a difficult Likelihood landscape for traditional MCMC: the initial position is on the wrong side of the barrier and is unlikely to jump over to the region of maximum Likelihood.

Sequential Monte Carlo addresses The difficulties by raising the Likelihood to a monotonically raising power, n =0..1. This flattens any barrier. Furthermore it uses many Markov chains to explore the space better.



Re-Sampling Posterior

To properly use Sequential Monte Carlo the various chains must be assigned a weight – a measure of how likely the region sampled by a chain is compared to another region. Their sum of all chains is normalized to one

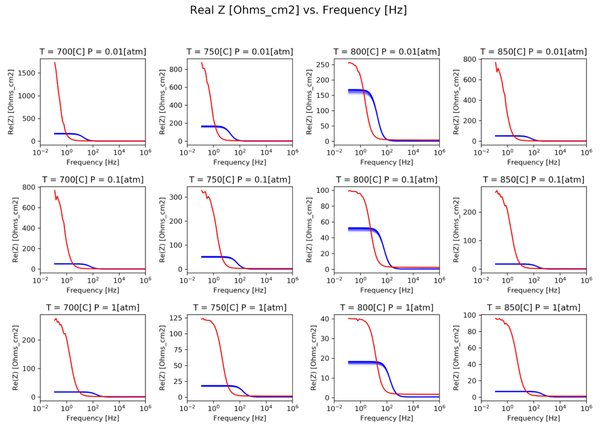


Within a chain each sample also has a weight. The sum of the samples is the weight of the normalized weight of the chain. Therefore, to reconstruct the posterior, we re-sample the results obtained using the SeqMCMC code. This is done by placing all chains and their samples along x-axis and drawing from a uniform distribution from zero to one.

SeqMC with Thin Film model

The first simulations to run a complete SeqMC run have completed. These runs had prior distribution tailored to make the run as stable as possible, therefore we expected the run result not to match the experimental values.

The model also has an improved model of the Schottky reaction that includes the stain energy of vacancy formation.



To improve the results above we are currently running broadened, more realistic, priors.

Conclusion

The Sequential Monte Carlo code and the analysis tool were developed to help explore large dimensional spaces with complicated surfaces. Currently we are using it to calibrate a Thin Film model; currently we are strengthening the reliability of the code to make large simulations possible.

Acknowledgement

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