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Quantifying Uncertainty of the Thermodynamic Efficiency of Redox Active Materials using Bayesian Inference

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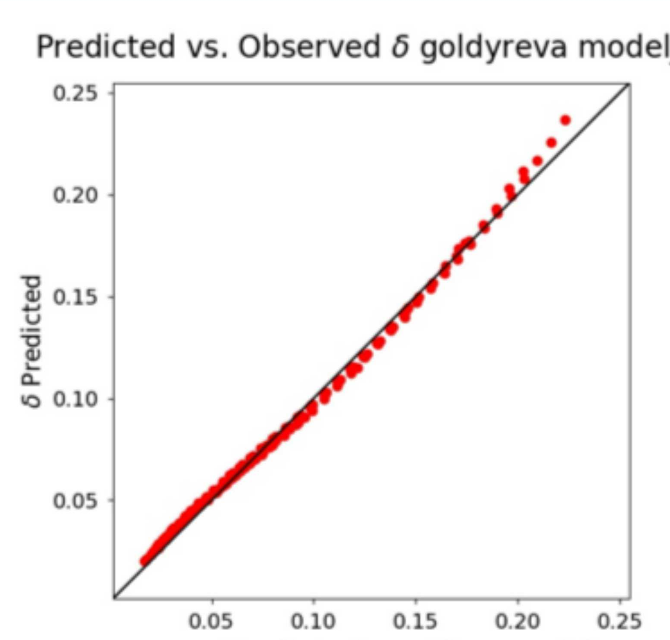
Purpose

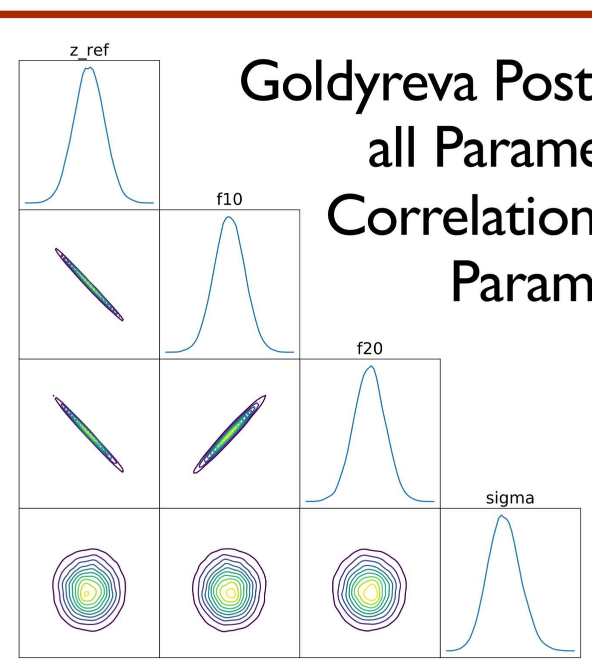
Finding a suitable functional redox material is a critical challenge to achieving scalable, economically viable technologies for storing concentrated solar energy in the form of a defected oxide. Demonstrating effectiveness for thermal storage or solar fuel is largely accomplished by using a thermodynamic model derived from experimental data. This portion of the project has three main goals:

- To assist the evaluation of newly developed materials used in Hydrogen conversion by calculating the confidence needed in the components that feed into the thermodynamic efficiency of this process in order to meet the desired accuracy.
- To improve the software engineering of the project, including making the code more robust, compatible with more models, and efficient.
- To develop a tutorial for the Uncertainty Qualification Toolkit (UQTk) to enable others to adapt these method to their projects.

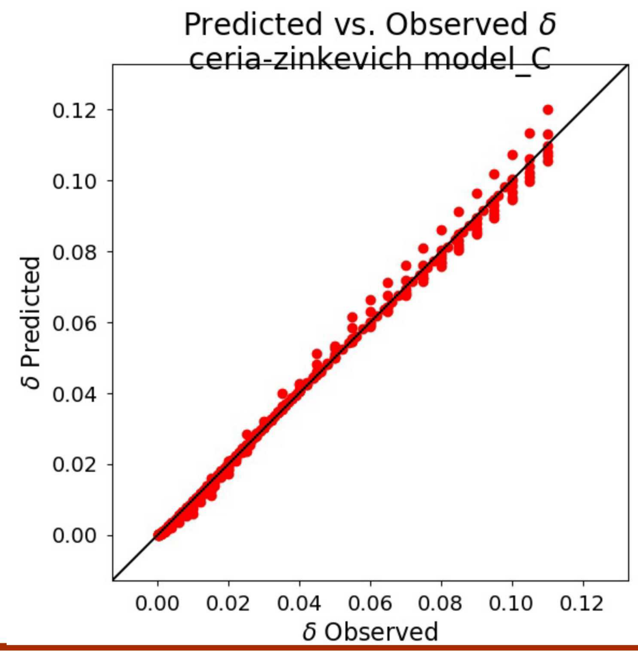
Approach

- Four models, with 3 – 7 parameters
  - Simplest model is linear
  - Most complicate is a quadratic divided by a quadratic
- Three data sets:
  - Zinkevich and Panlener: from a material used for solar fuels by splitting water and carbon dioxide
  - Goldyreva: from a material for thermal storage

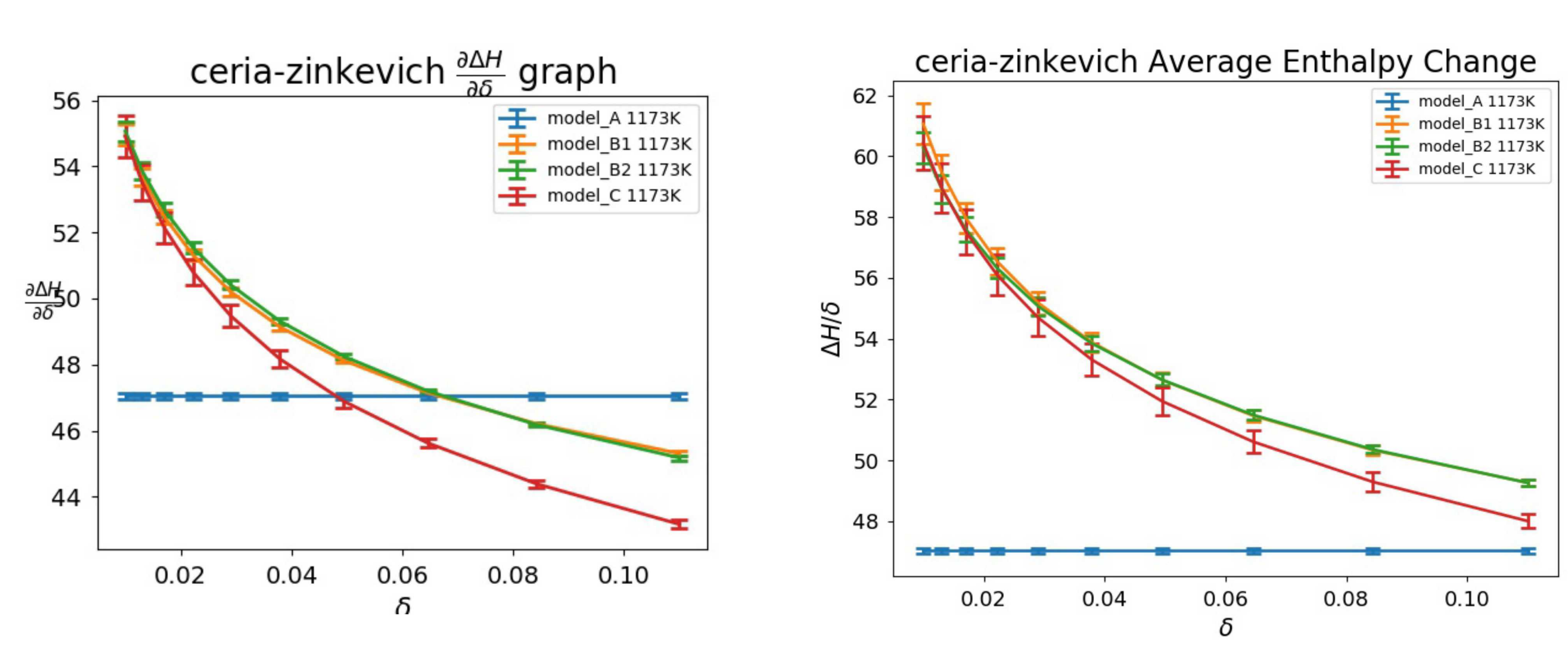




Goldyreva Posterior Plots for all Parameters and Correlations Between Parameters



The model fit for various data sets and models. They display the observed δ vs the predicted δ with the black line showing the ideal fit. The parameters for the models were determined using Markov Chain Monte Carlo (MCMC), posterior plots and correlations between parameters shown above.



These graphs show the enthalpy. The left graph shows the enthalpy derivative and the right graph shows the averaged enthalpy change. The error bars show the uncertainty in the calculations, and were determined using Monte Carlo sampling. MCMC produces a posterior distribution of the most likely parameters, which we can use to determine the uncertainty in physical quantities like enthalpy.

Next steps:

- To calculate the model efficiency, including the uncertainty
- To propagate uncertainties through the model to determine how accurate the initial experiments need to be in order to calculate efficiency with a desired accuracy
- To analyze other models, variations of current models

Software Engineering

Part of this summer's work includes improving current software engineering. This includes making the codes:

- More adaptable to new methods
  - Current models are substantially different in format from old models; want robust enough code to handle different models
  - Planning to change models, introduced slight variations on models, and possible completely different model.
- More efficient
  - Currently implemented in Python; change some components to C++, many of which are already implemented in UQTk
  - Possibly run on multiple cores for multiple models

Tutorial

Another component of this project is to make this analysis available to other scientists as part of the Uncertainty Quantification Toolkit (UQTk). Thus, the codes need to be written with generalization in mind, so that others can easily adapt this code to their specific problem. Planning to finish tutorial this summer, and release tutorial in the fall update of UQTk.

Acknowledgments

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