Reduced-order model for microstructure evolution simulation in solid oxide fuel cell with dynamic discrepancy reduced modeling

Yinkai Lei [a, b], Tian-Le Cheng [a, c], Harry Abernathy [a, d], Gregory Hackett [a], David Mebane [a, c], You-Hai Wen [a]

[a] US DOE National Energy Technology Laboratory, Albany, OR [b] Oak Ridge Institute for Science and Education, Oak Ridge, TN [c] Leidos Research Support Team, Albany, OR

[d] Leidos Research Support Team, Morgantown, WV [c] Department of Mechanical and Aerospace Engineering, West Virginia University, Morgantown, WV

Research & Innovation Center

NATIONAL ENERGY TECHNOLOGY LABORATORY

Background

- Microstructure evolution in SOFC anode due to Ni coarsening leads to loss of TPB density, specific surface area and electronic conductivity.
- Phase field models have been developed to model the microstructure evolution in SOFC anode [1]. But they are expensive: typical length scale is only ~10 μm in each dimension, typical time scale is <1000 hours at 1000 ºC in two days.
- A reduced-order model that is much faster than the phase field model but with similar accuracy is needed.

Model Building Strategy

- State variables: moments of particle size distribution

  Average Ni radius: $\langle r \rangle = \int rp(r)dr$

  Standard deviation: $\sigma^2 = \int r^2 p(r)dr - \langle r \rangle^2$

  Reduction of model order: from ~1 million in phase field model to 2.
- Kinetic equations from the theory of Ostwald ripening.

$$\frac{d\langle r \rangle}{dt} = \frac{K(A_2 - A_1)}{2RT\langle r \rangle^2}$$

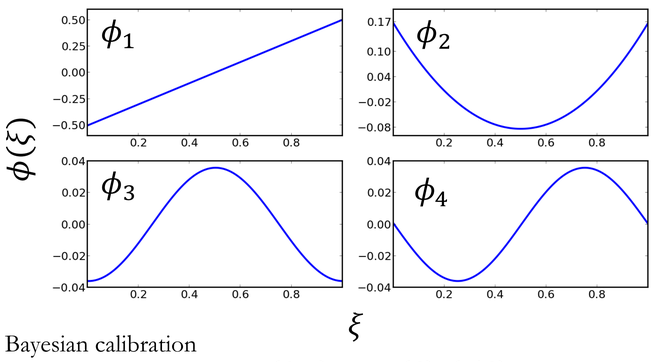
$$\frac{d\sigma}{dt} = \frac{K}{RT\langle r \rangle \sigma}\left[(1 - A_1) + \frac{3\sigma^2 + 4\langle r \rangle^2}{4\langle r \rangle^2}(A_2 - A_1)\right]$$

  Property models are developed from percolation theory [2].
- Dynamic discrepancy function [3]

$$P = P_0 \exp[\delta(\langle r \rangle, \sigma, f_{Ni}, f_{YSZ})],\ P = K, A_1, A_2, \ldots$$

  $\delta(\boldsymbol{\xi})$ is a Gaussian Process parameterized by a set of basis functions:

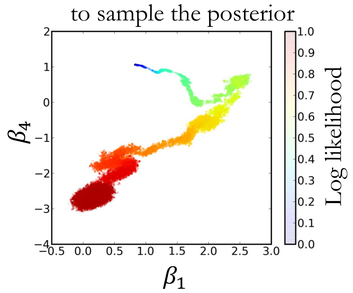
$$\delta(\xi;\beta) = \beta_0 + \sum_{ij}\beta_j^i \phi_j(\xi_i) + \sum_{ijkl}\beta_{jl}^{ik}\,\phi_j(\xi_i)\phi_l(\xi_k) + \cdots$$



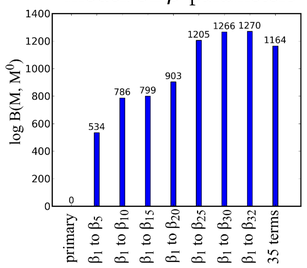
- Bayesian calibration

$$p(\theta|y) = \frac{p(\theta, y)}{p(y)} = \frac{p(\theta)p(y|\theta)}{\int p(\theta)p(y|\theta)d\theta}$$

Markov chain Monte Carlo method to sample the posterior

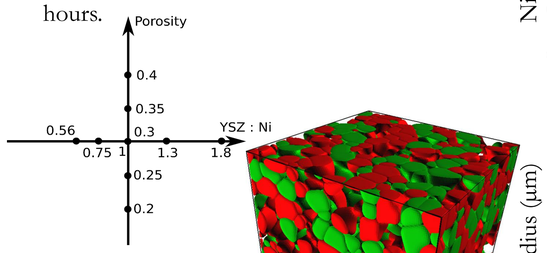


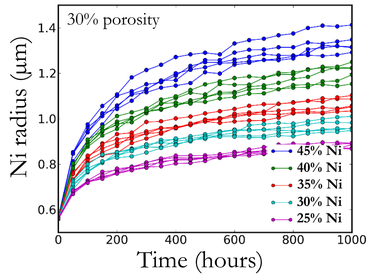
Bayes factor to identify the best model: 32 β parameters

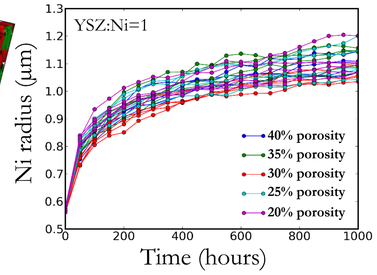


Data Generation

- 9 different compositions with 5 initial microstructures for each composition.
- 12.8 microns in each dimension with voxel size of 0.1 micron
- Phase field simulations at 1000 ºC up to 1000 hours.



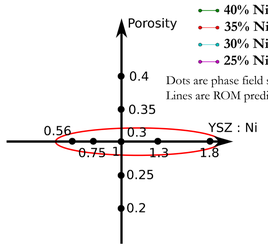


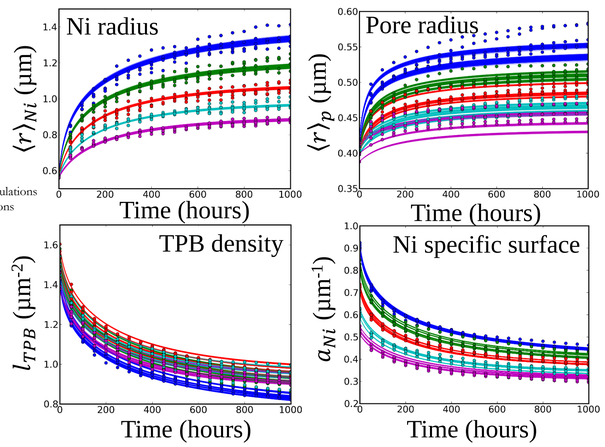


Results & Application

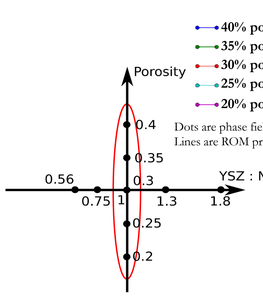
- **Results:** calibrated model

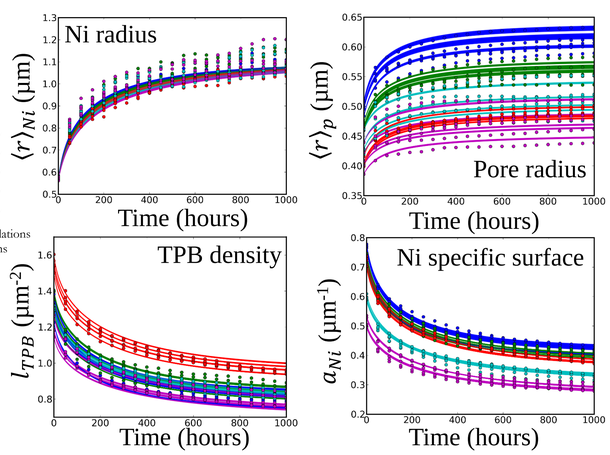
30% porosity



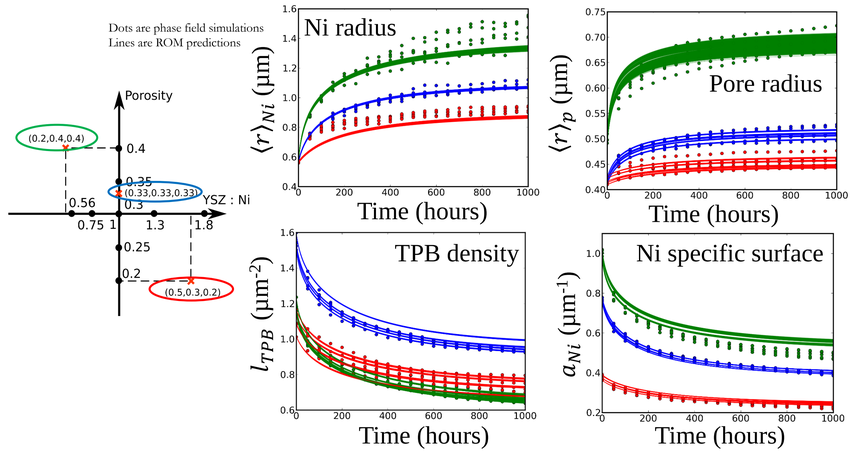


YSZ:Ni=1

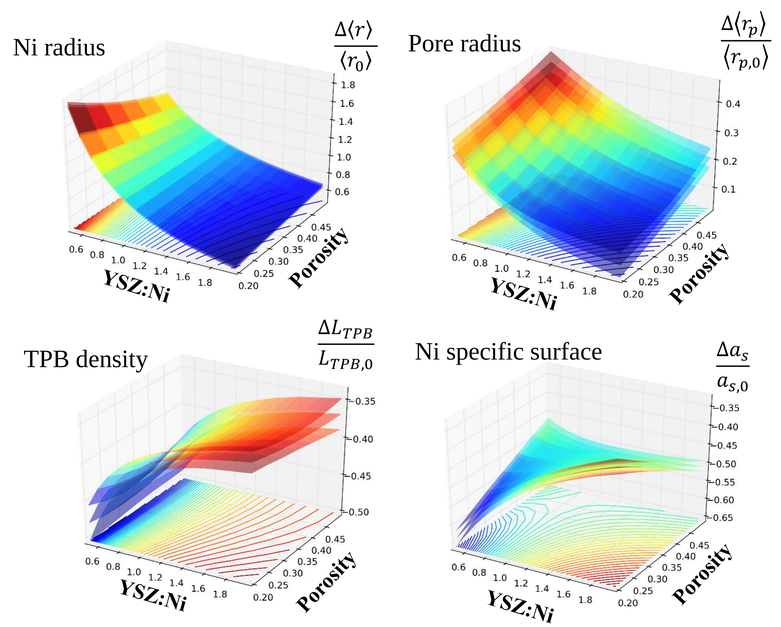




- **Results:** model validation



- **Application:** microstructure evolution maps, relative property change after 10,000 hours.



Conclusions

- A reduced order model has been built by inserting dynamic discrepancy function into the kinetic equations of Ostwald ripening. The calibrated model well resembles the prediction of phase field simulations.
- The calibrated model predicts that increasing the YSZ volume fraction and reducing the porosity slows down the Ni coarsening in SOFC anode.

References: [1] Lei et al, J Power Sources, 345, 275-289 (2017); Liang et al, J. Appl. Phys, 117, 065105 (2015). [2] Mason et al, J Electrochem Soc, 165, F64-74 (2018) [3] Li et al, React. Chem. Eng., 2, 550 (2017)

Acknowledgement:
The authors would like to thank Drs. Long-Qing Chen, Paul Salvador, William Epting, Jerry Mason, Giuseppe Brunello and Tom Kalapos for valuable technical discussions. 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.

Science & Engineering To Power Our Future