Multi-component Gas Transport in a Solid Oxide Fuel Cell Anode using the Lattice Boltzmann Method

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Presentation for ESI CFD Inc. (Huntsville, AL)
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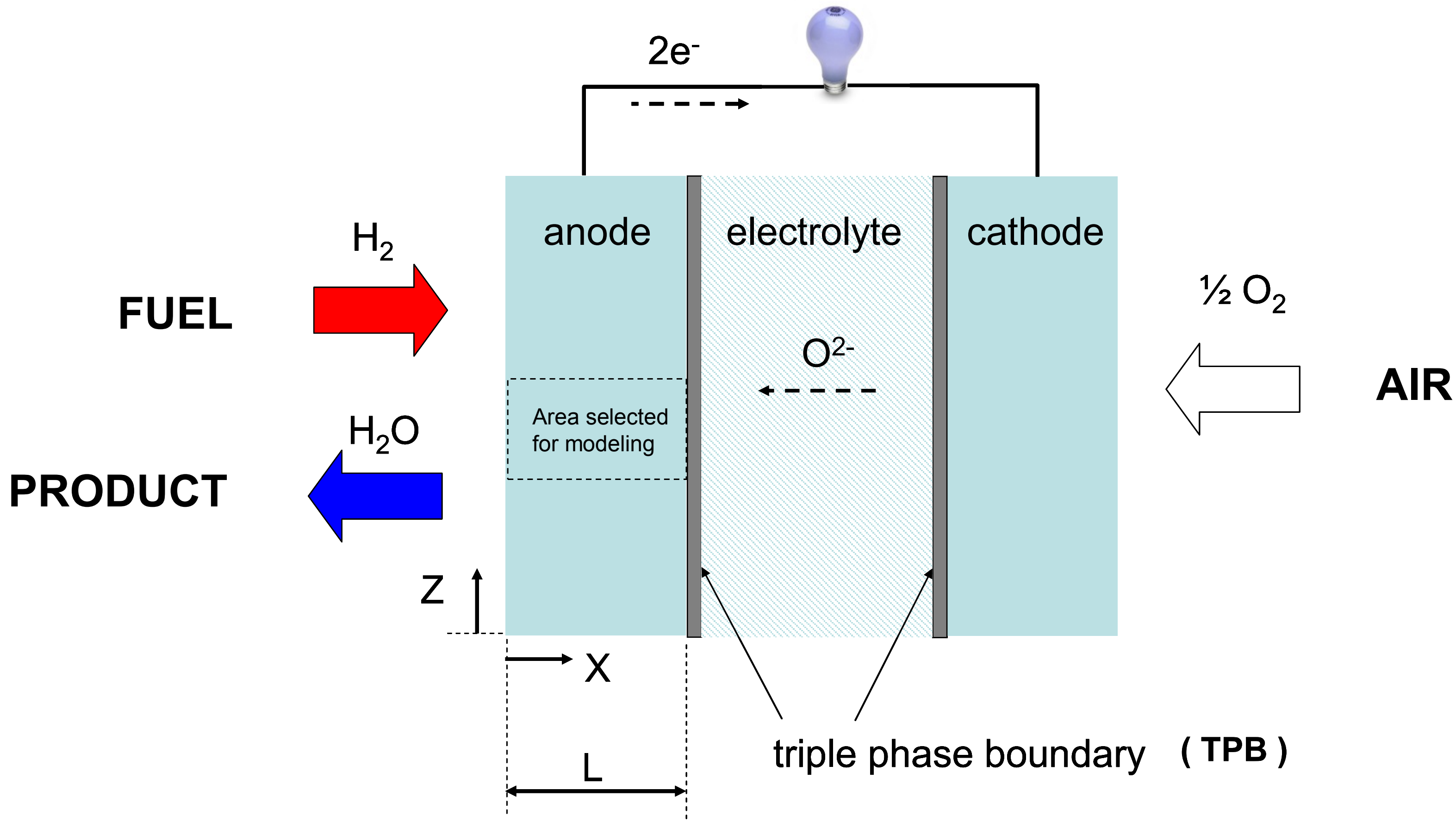
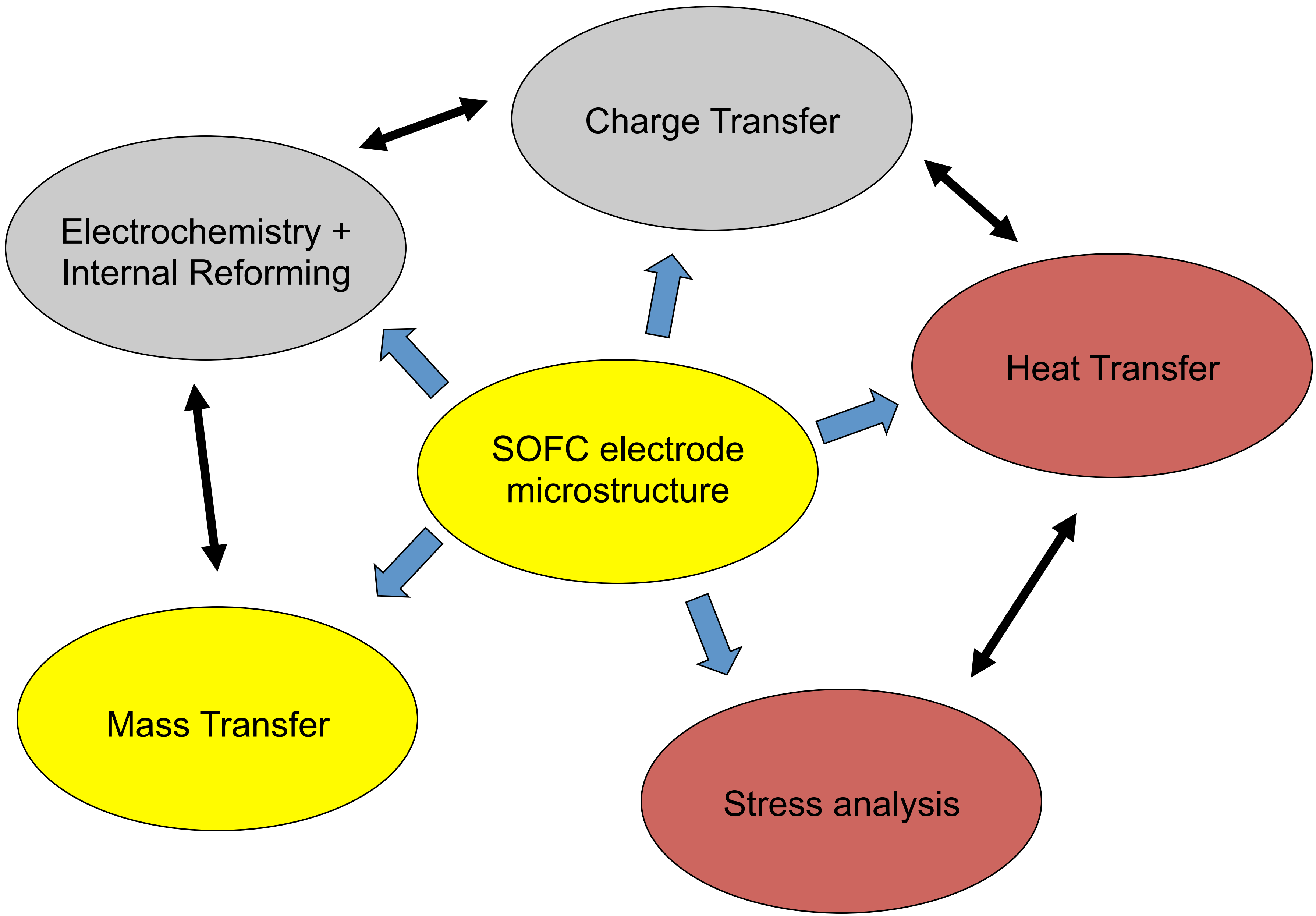
Introduction to SOFC

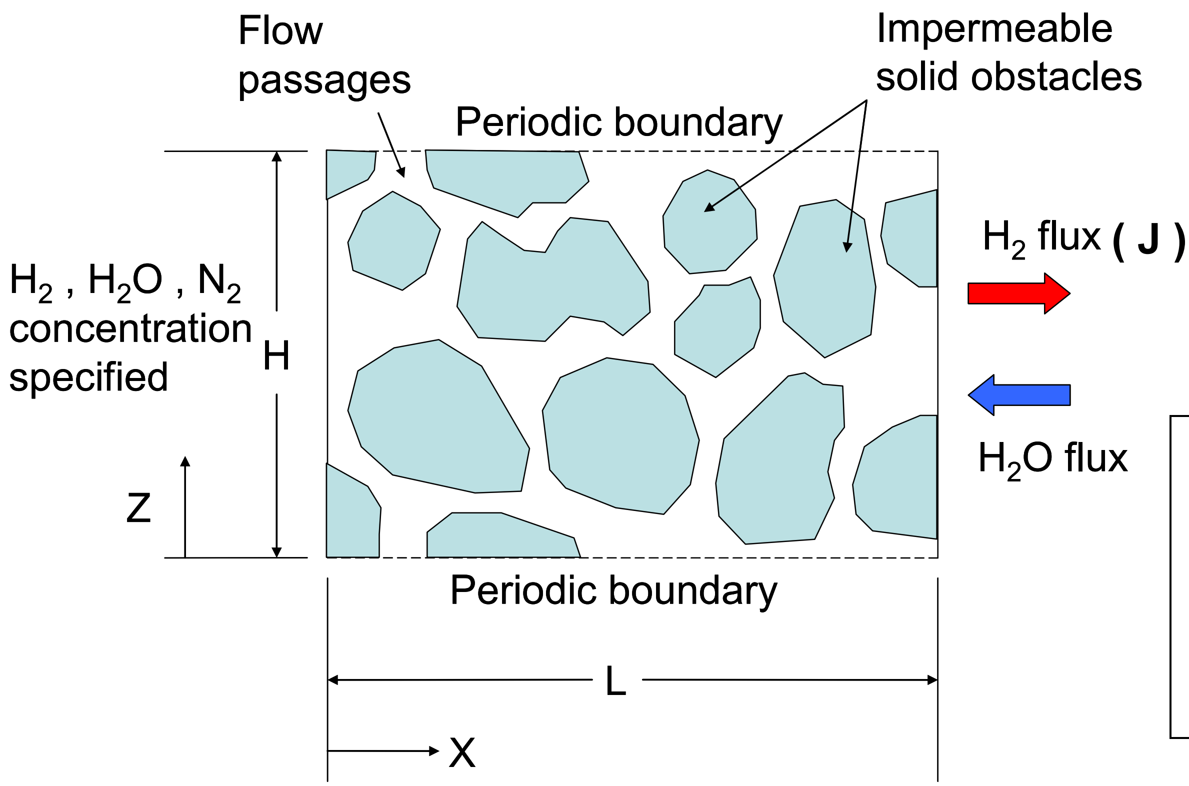


- ❑ Need to accurately model mass transport of fuel (H_2) and product (H_2O) in the porous anode.
- ❑ Anode geometry can be optimized to improve SOFC performance

SOFC: Developing a Comprehensive Model



Mass Transport Model for a SOFC Anode



Dimensionless current density

$$J^* = \frac{J\ L}{C_T\ D_{23}}$$

Porosity

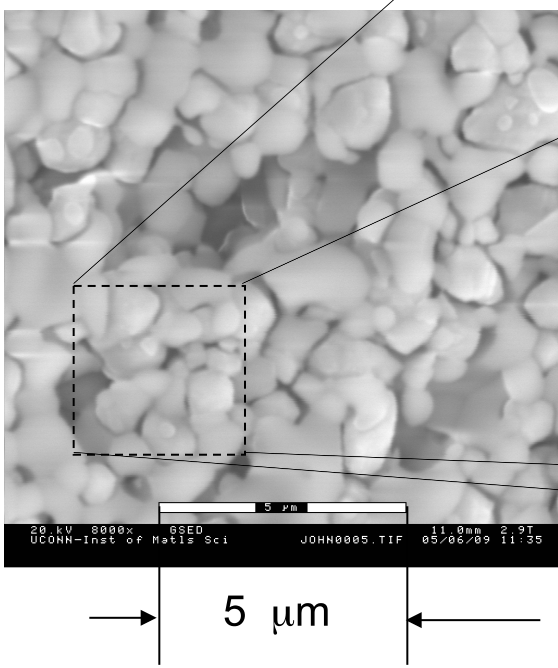
$$\phi = \frac{Area\ of\ void\ space}{Total\ area}$$

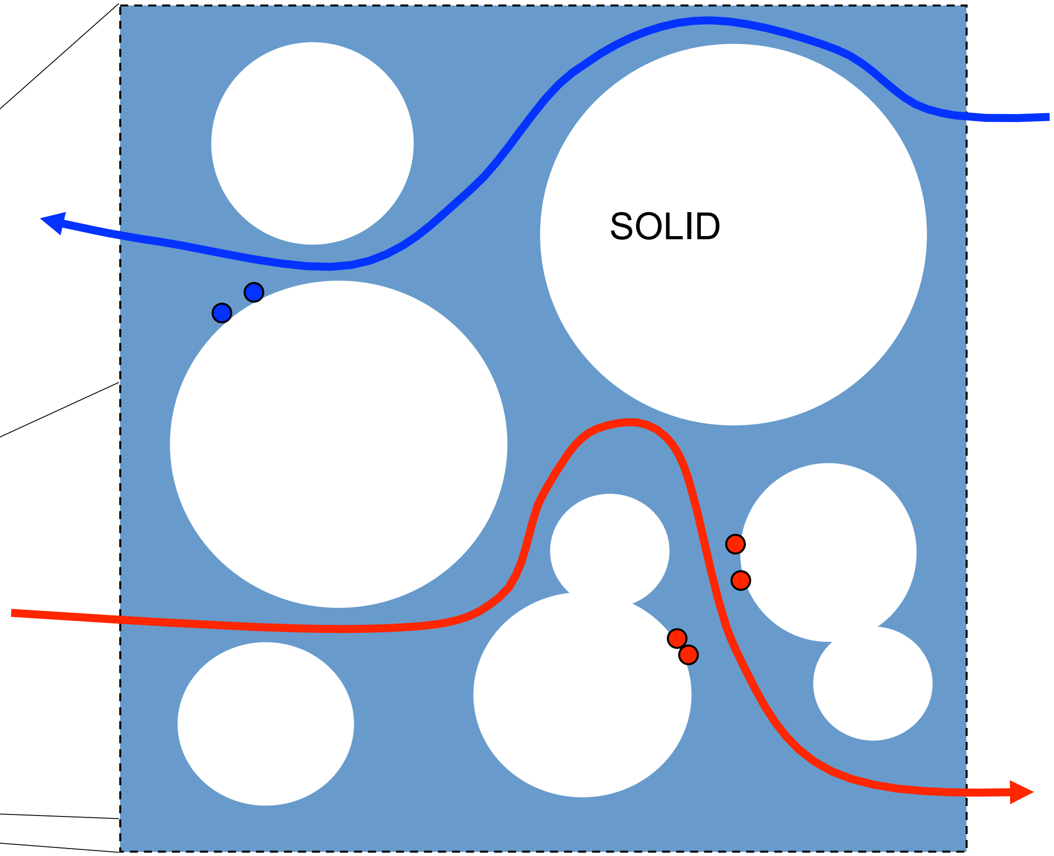
- ❑ Species concentration is specified at the gas channel.
- ❑ Mole flux of H_2 and H_2O is specified at the TPB.
- ❑ Mole flux of the inert species (N_2) at the TPB is zero.

Modeling Challenges

Gas diffusion occurs at high temperature and through micron size pores. Continuum theory is no longer valid.

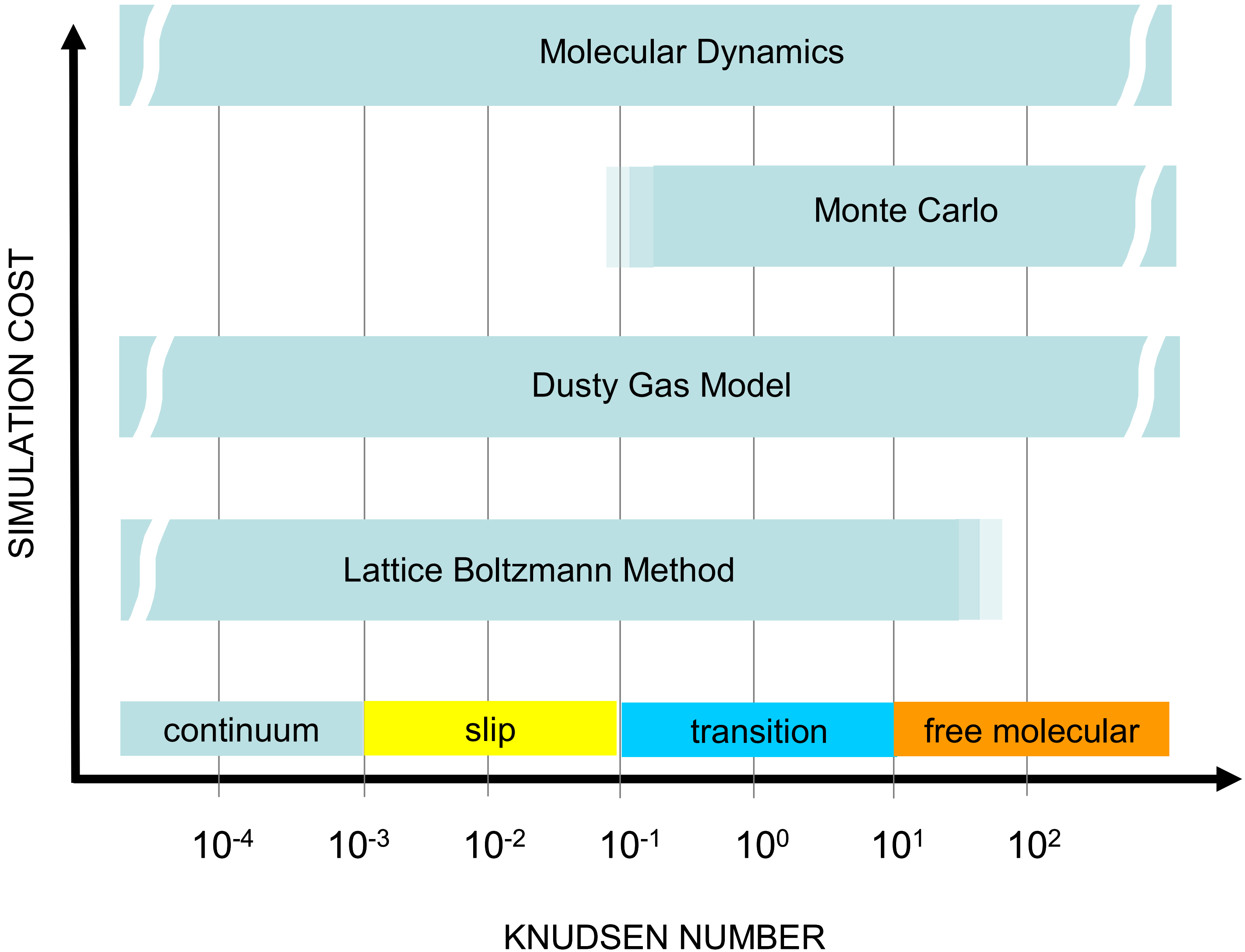
Gas particles can get adsorbed on the solid material of the anode





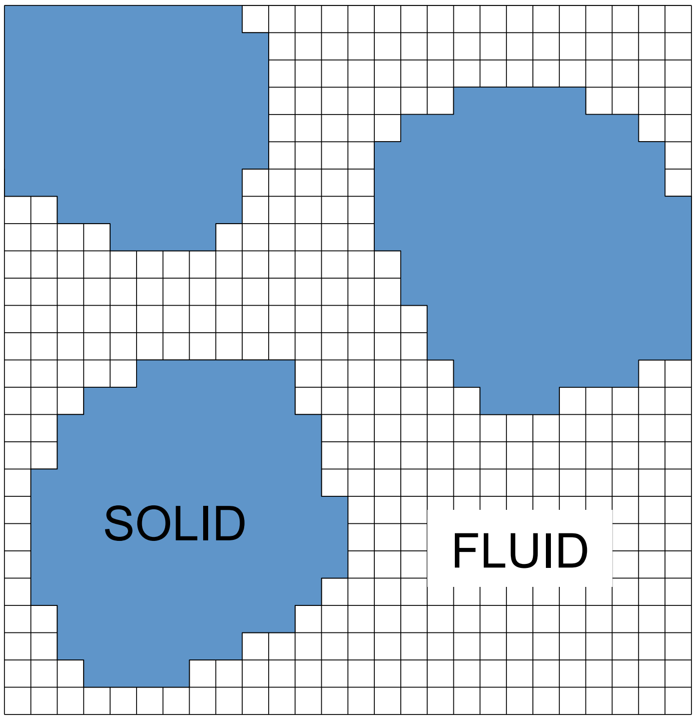
Chemical reactions among gas components need to be included for the case of internal reforming and at the TPB.

Comparison of Modeling Approaches



Lattice Boltzmann Method (LBM)

- Historically derived from the lattice gas cellular automata
- LBM is a numerical approximation to the Boltzmann equation



Desirable Features

- Multiple species
- Complex geometry
- Parallel algorithm
- Wall interactions
- Non-continuum regime

Basic LBM Algorithm: Stream and Collide

new time level

species

old time-level

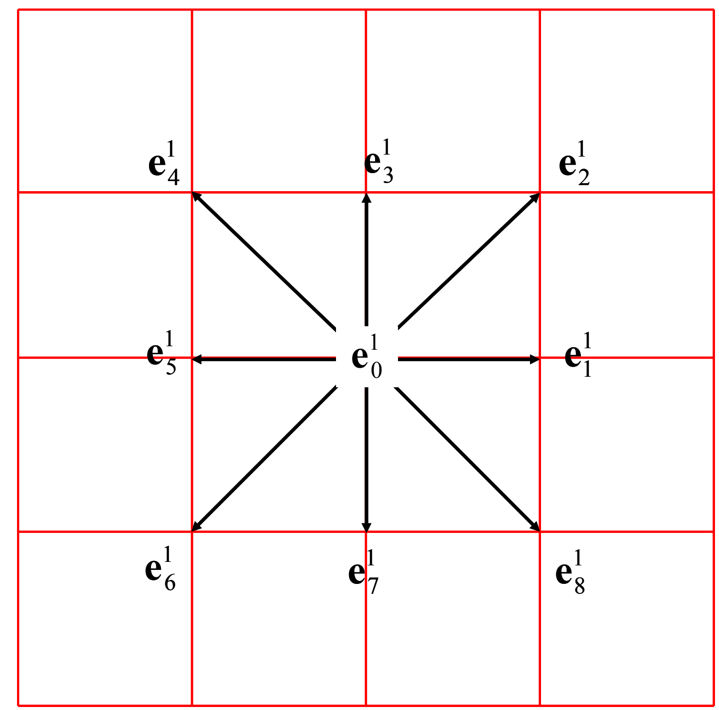
$$f^{\sigma,\,n+1}_{i,\mathbf{r}+\mathbf{e}_i} = f^{\sigma,\,n}_{i,\mathbf{r}} - \Omega^{\sigma,\,n}_{i,\mathbf{r}}$$

discrete velocity

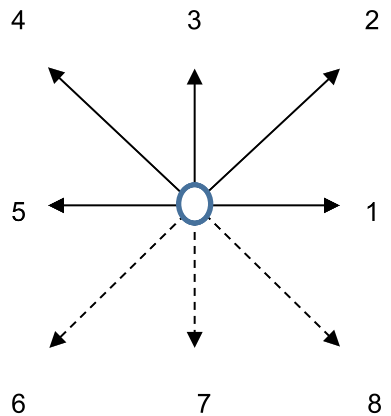
direction

velocity distribution function

BGK collision term



Bounce Back Boundary Condition



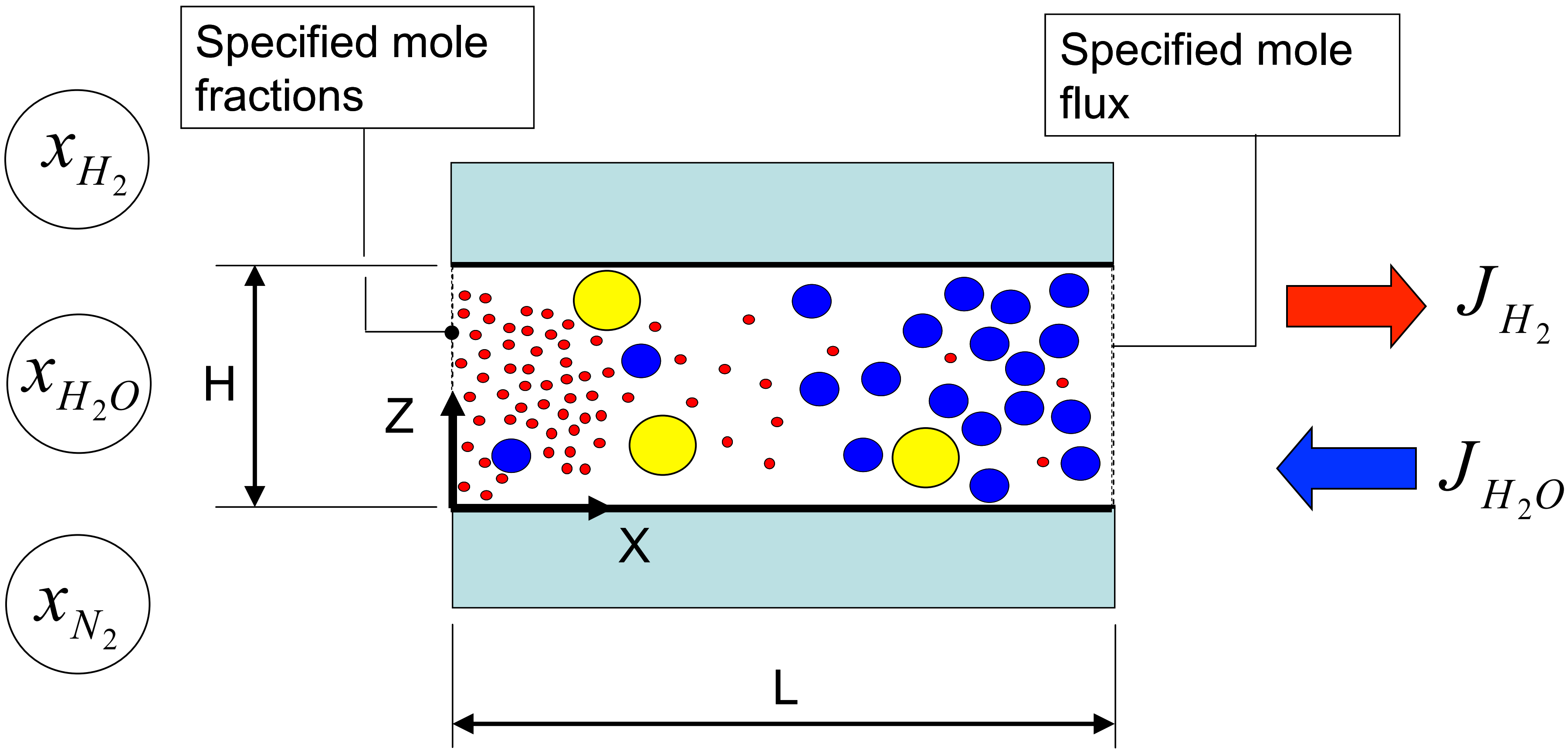
$$f_6 = f_2$$

$$f_7 = f_3$$

$$f_8 = f_4$$

Bounce back condition simulates no-slip at solid walls.

LBM Validation – Problem Definition



Equimolar counter-diffusion of H_2 and H_2O is assumed.

$$J_{H_2} = -J_{H_2O} = J$$

1-D Stefan-Maxwell Gas Transport Model

$$\frac{d\left(x_1 C_T\right)}{dx} = -\left[\frac{x_1 + x_2}{D_{12}} + \frac{x_3}{D_{13}}\right] J$$

$$\frac{d\left(x_2 C_T\right)}{dx} = +\left[\frac{x_1 + x_2}{D_{21}} + \frac{x_3}{D_{23}}\right] J$$

$$\frac{d\left(x_3 C_T\right)}{dx} = +x_3 \left[\frac{1}{D_{13}} - \frac{1}{D_{23}}\right] J$$

Fick's law of diffusion is obtained as a special case for a **binary** system.

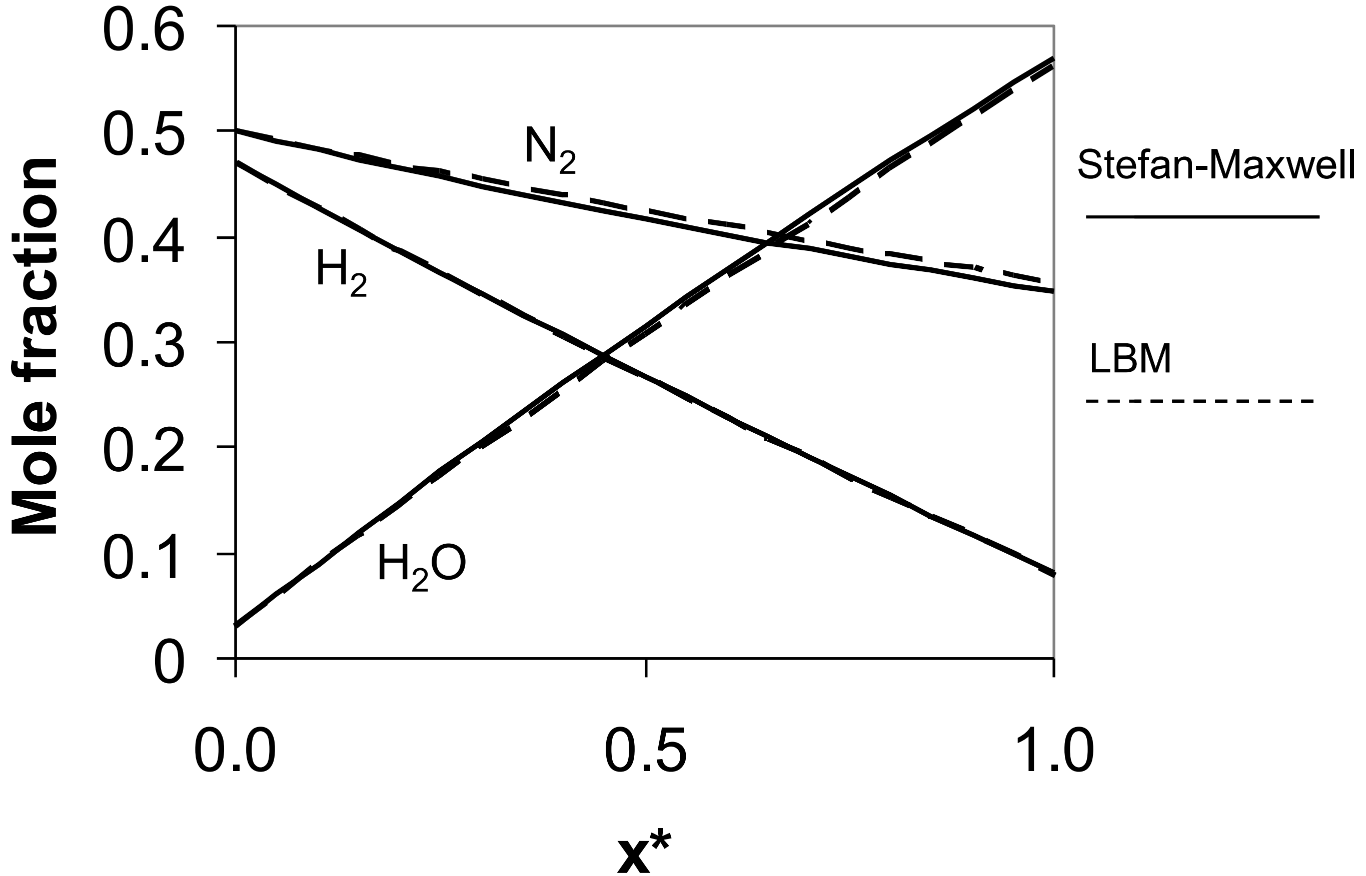
- ❑ The desired output is the species mole fraction profiles
- ❑ The Stefan-Maxwell equations are solved numerically
- ❑ Total concentration is a constant in the continuum regime

LBM Validation - Results

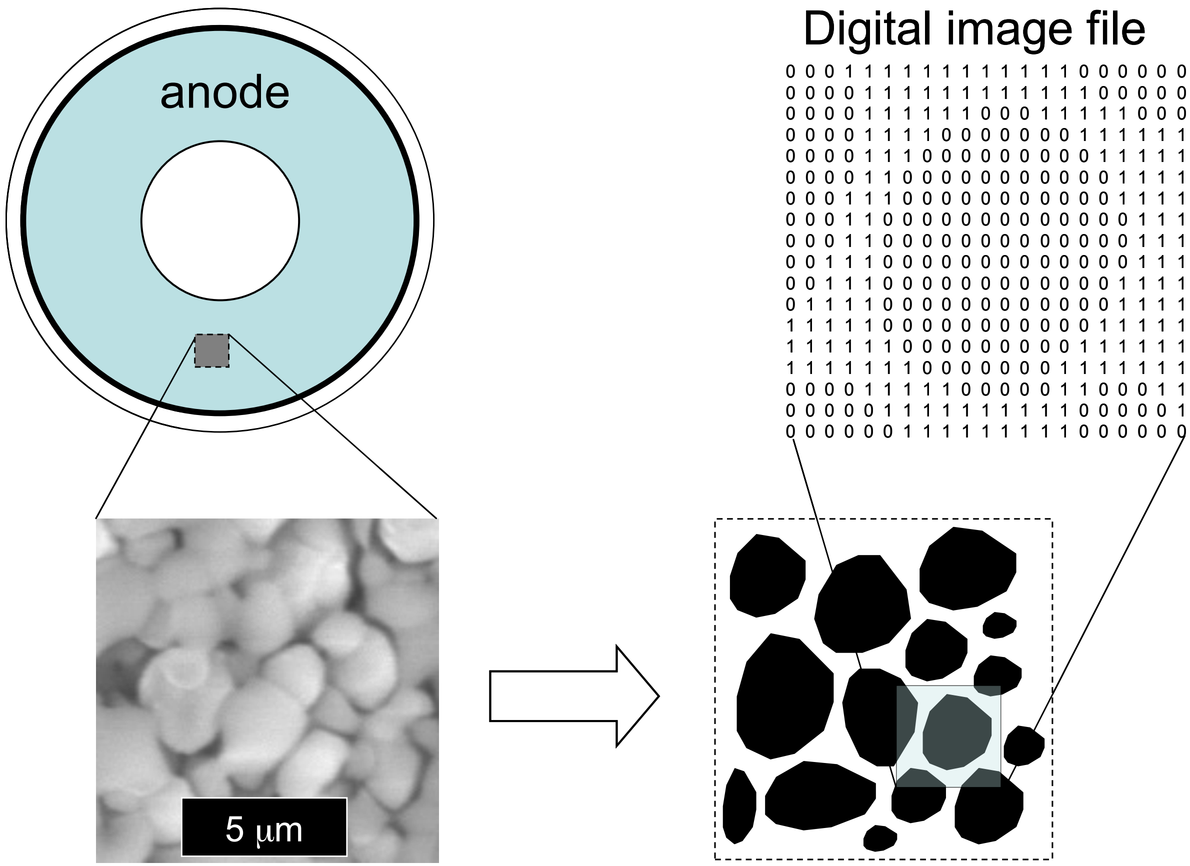
J* = 0.64

Specified mole fractions at the left boundary

H_2	0.47
H_2O	0.03
N_2	0.50



2D Image Processing using SEM



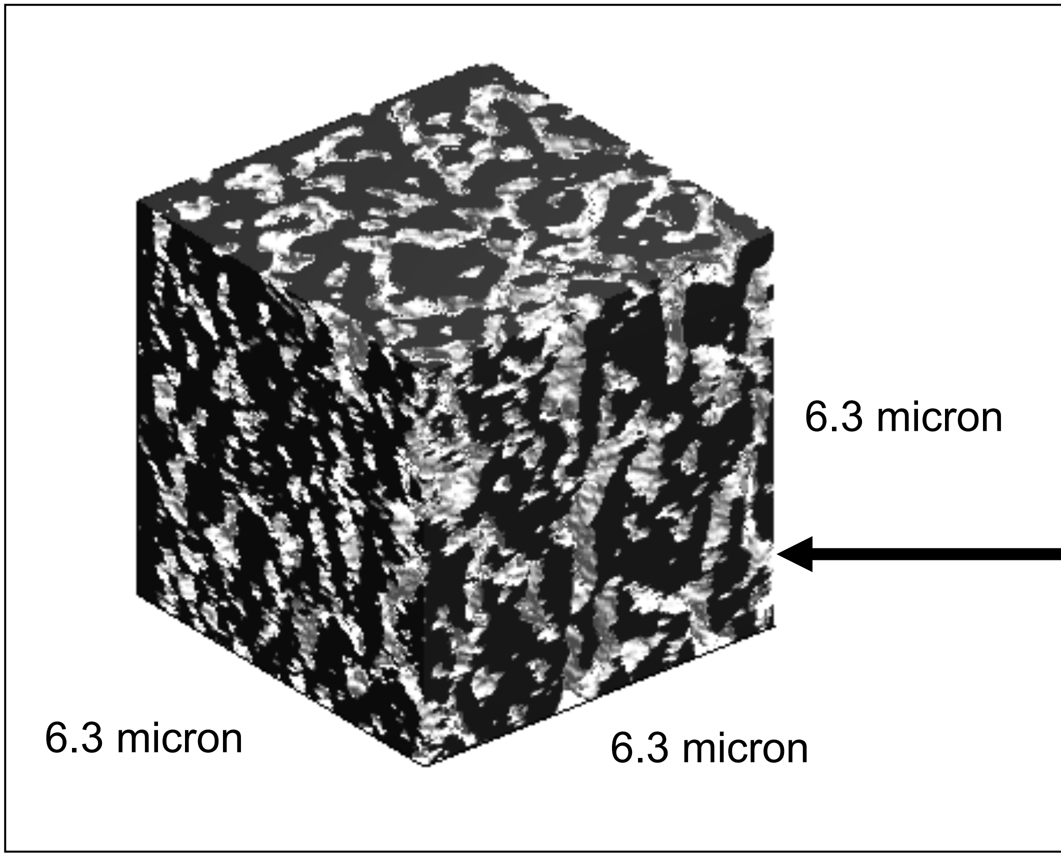
Actual SEM image

Model Image

ImageJ is used for converting the model image to digital form.

http://rsb.info.nih.gov/ij/

3D Geometry Reconstruction using XCT



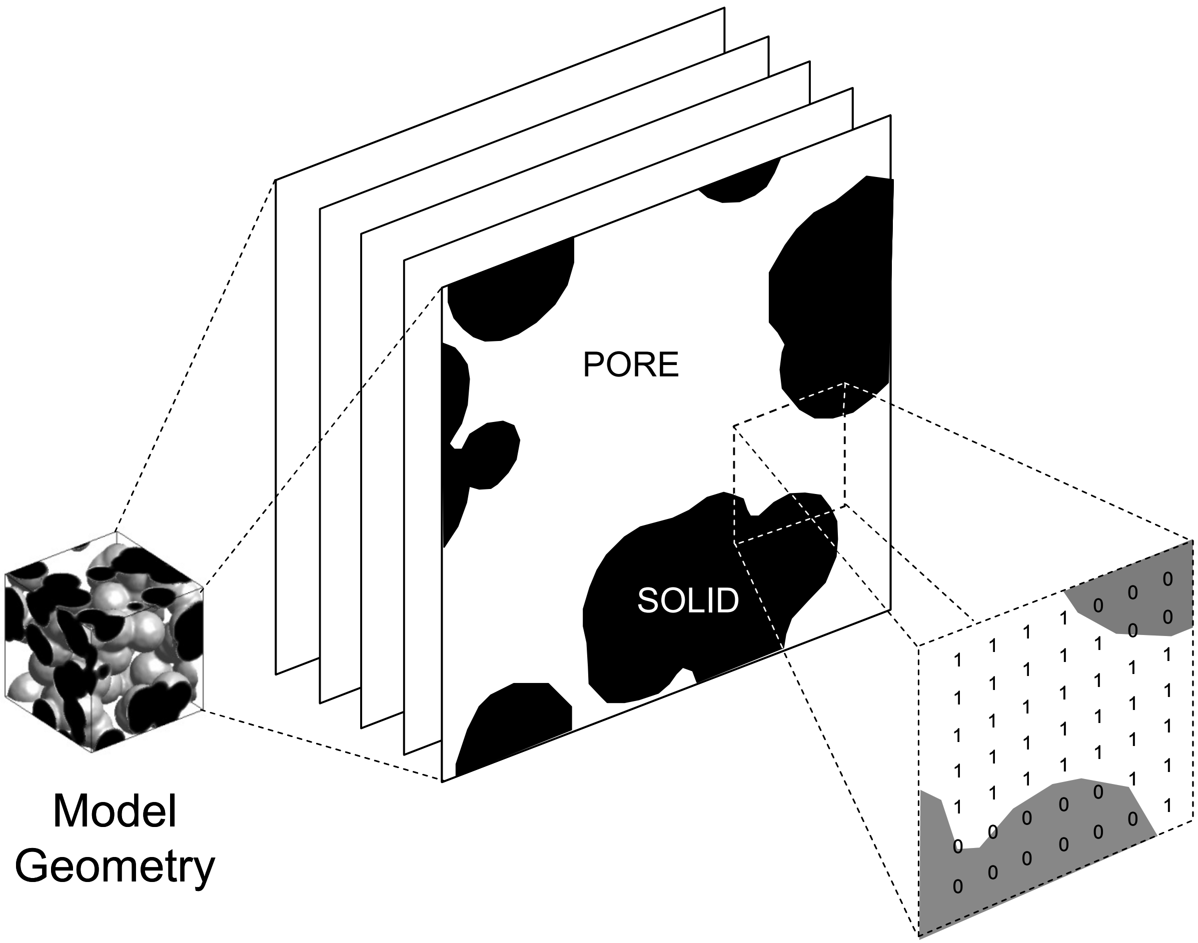
Non-destructive method

< 50 nm resolution

Dark area: **solid**

Bright area: **pore**

3D Image Processing on a slice-by-slice Basis

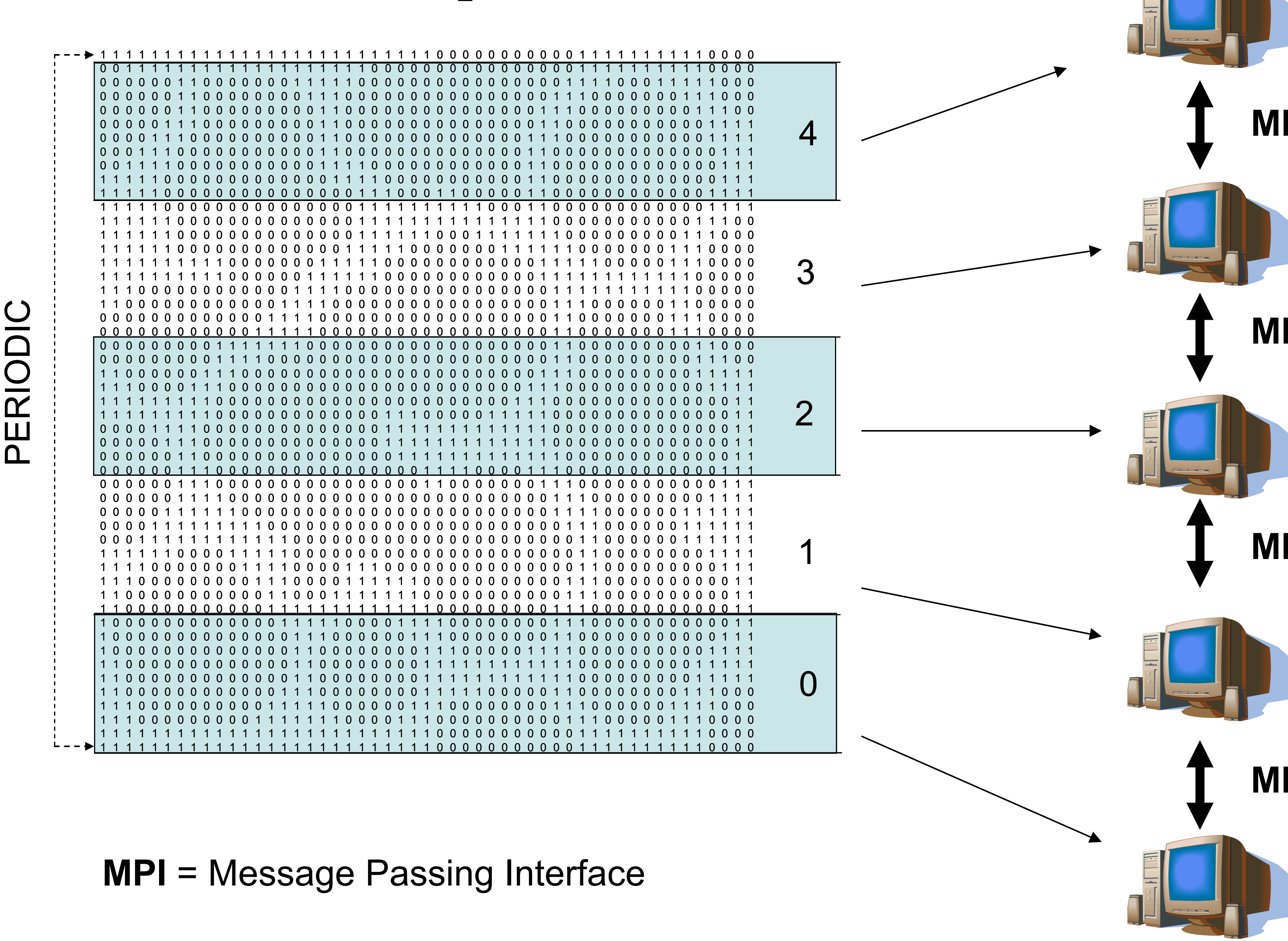


Model Geometry

Binary Representation

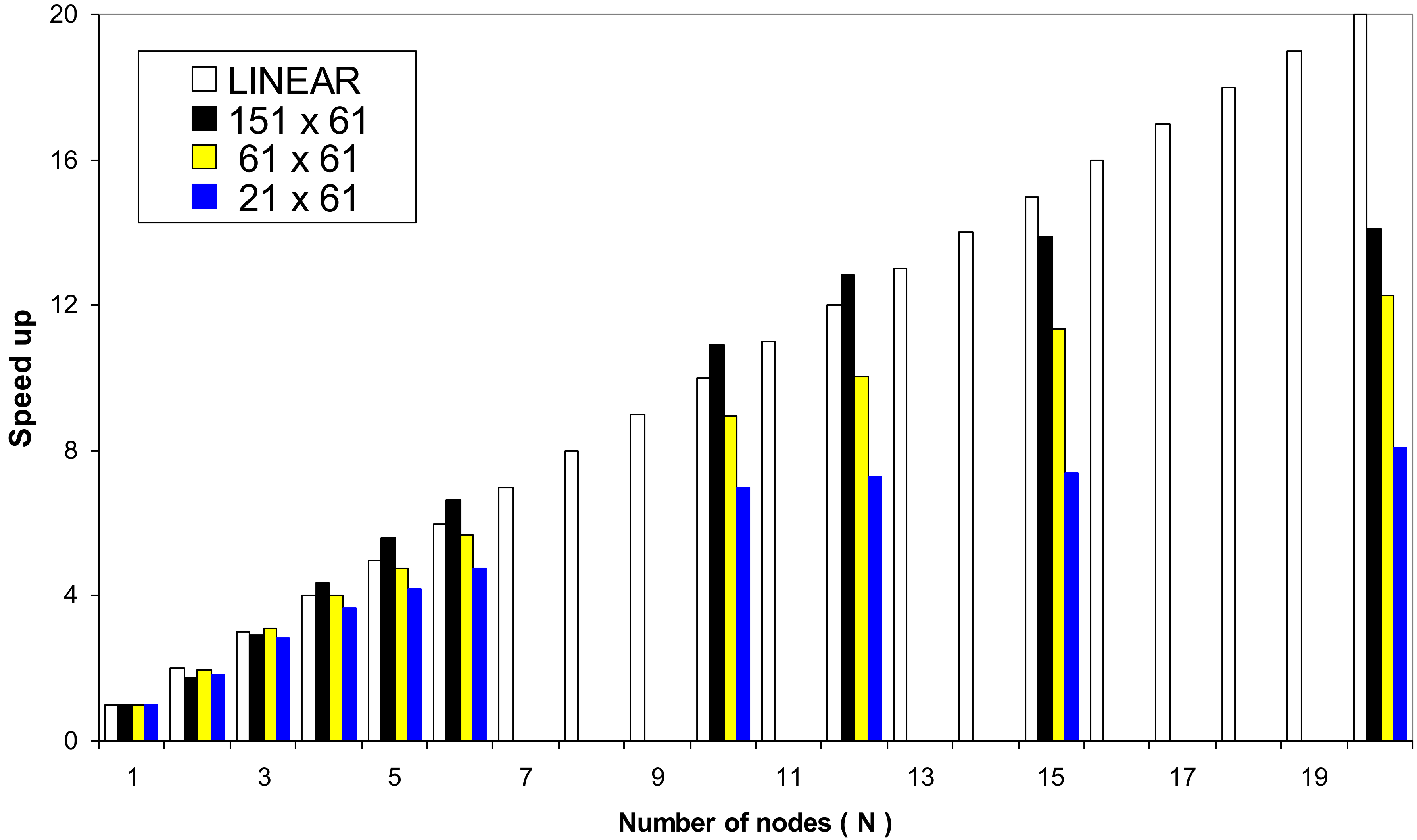
ImageJ used to create binary representation

Parallel Implementation of the LBM



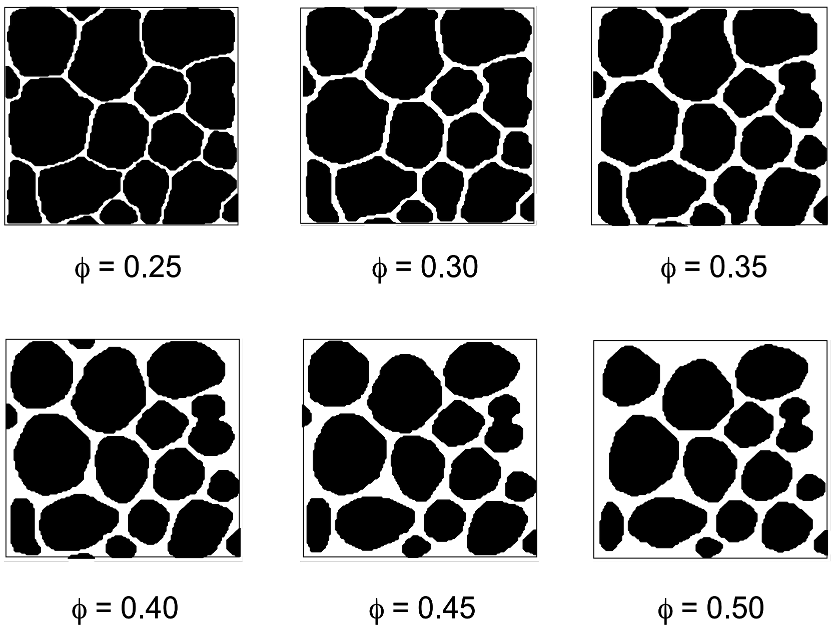
MPI = Message Passing Interface

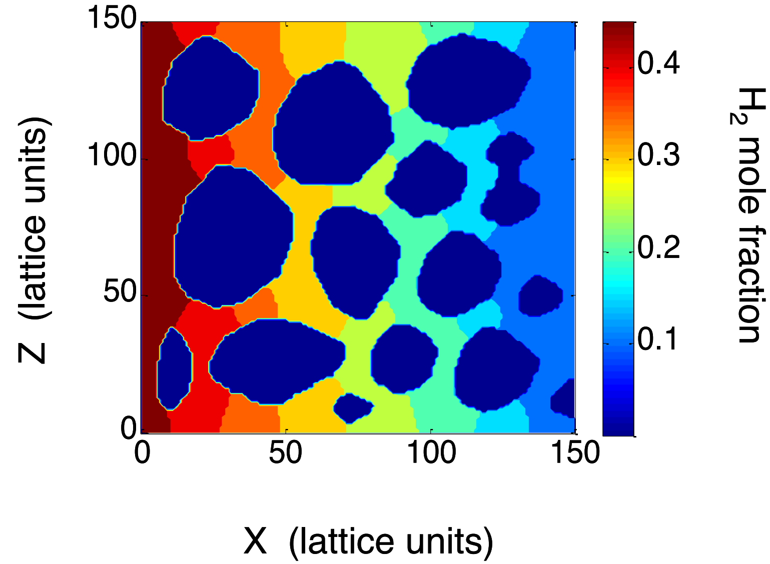
Parallel Performance of the LBM

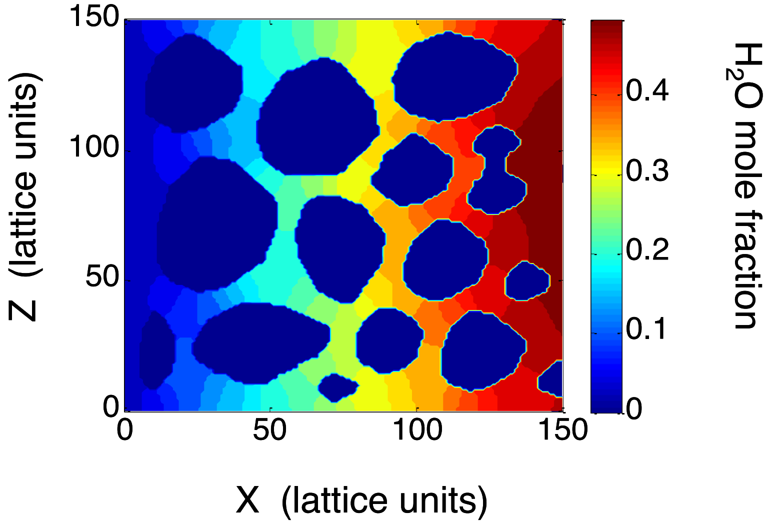


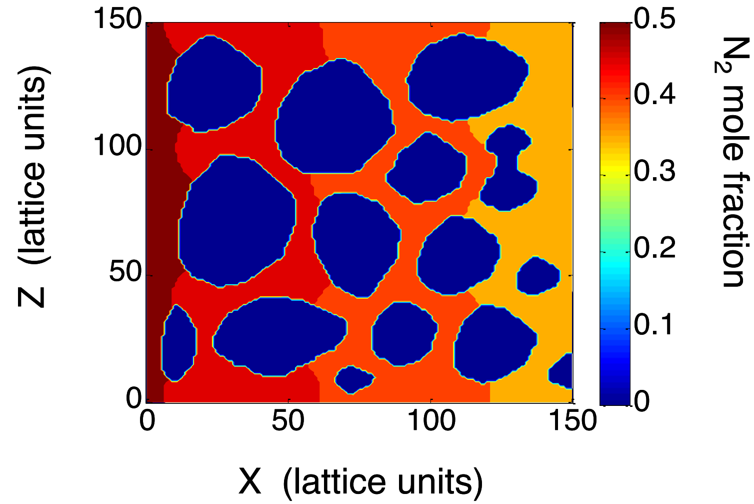
For N = 1, run times were: 10 hrs 38 min 36 min 88 sec

Anode Geometry and Mole Fraction Distribution

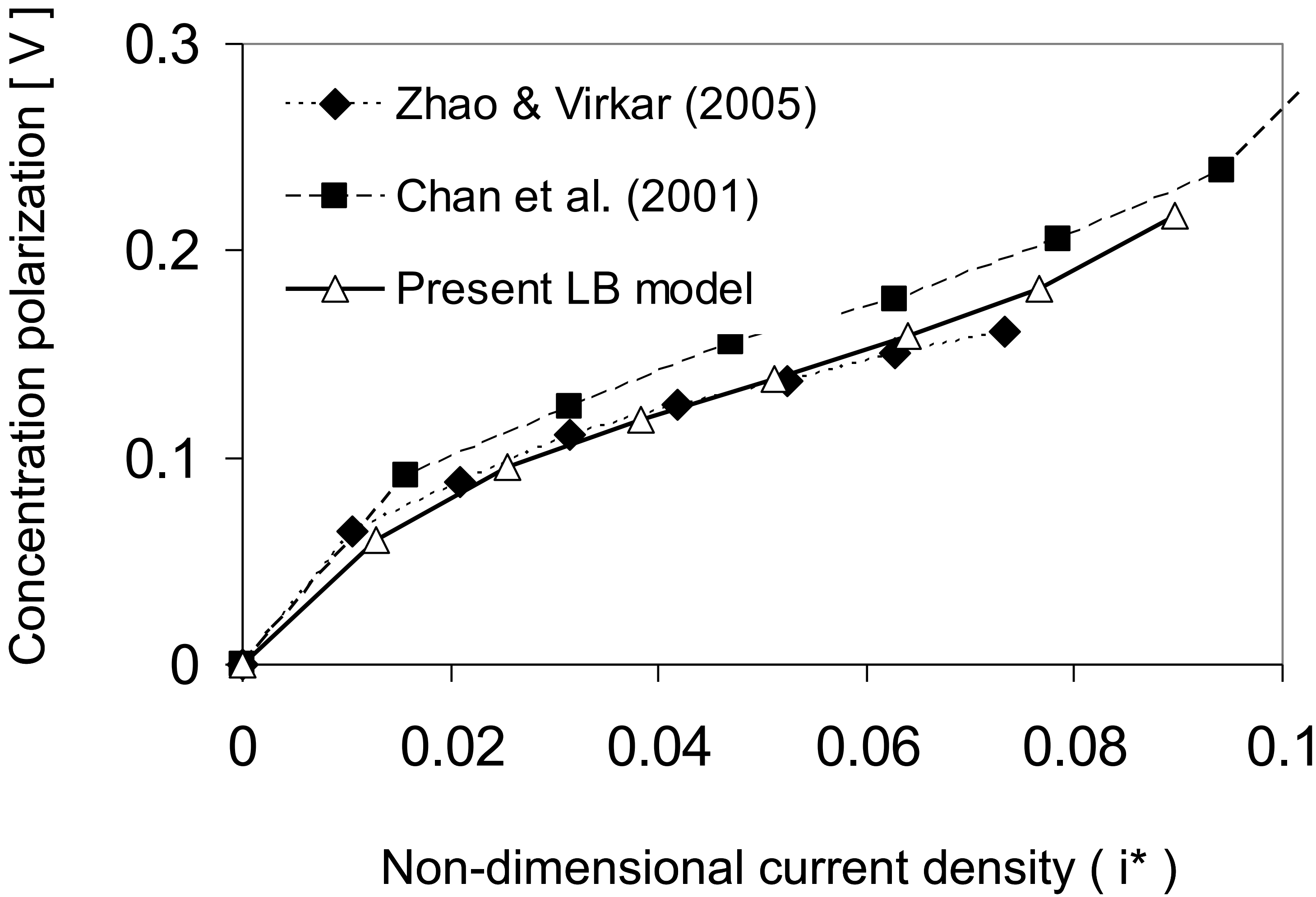




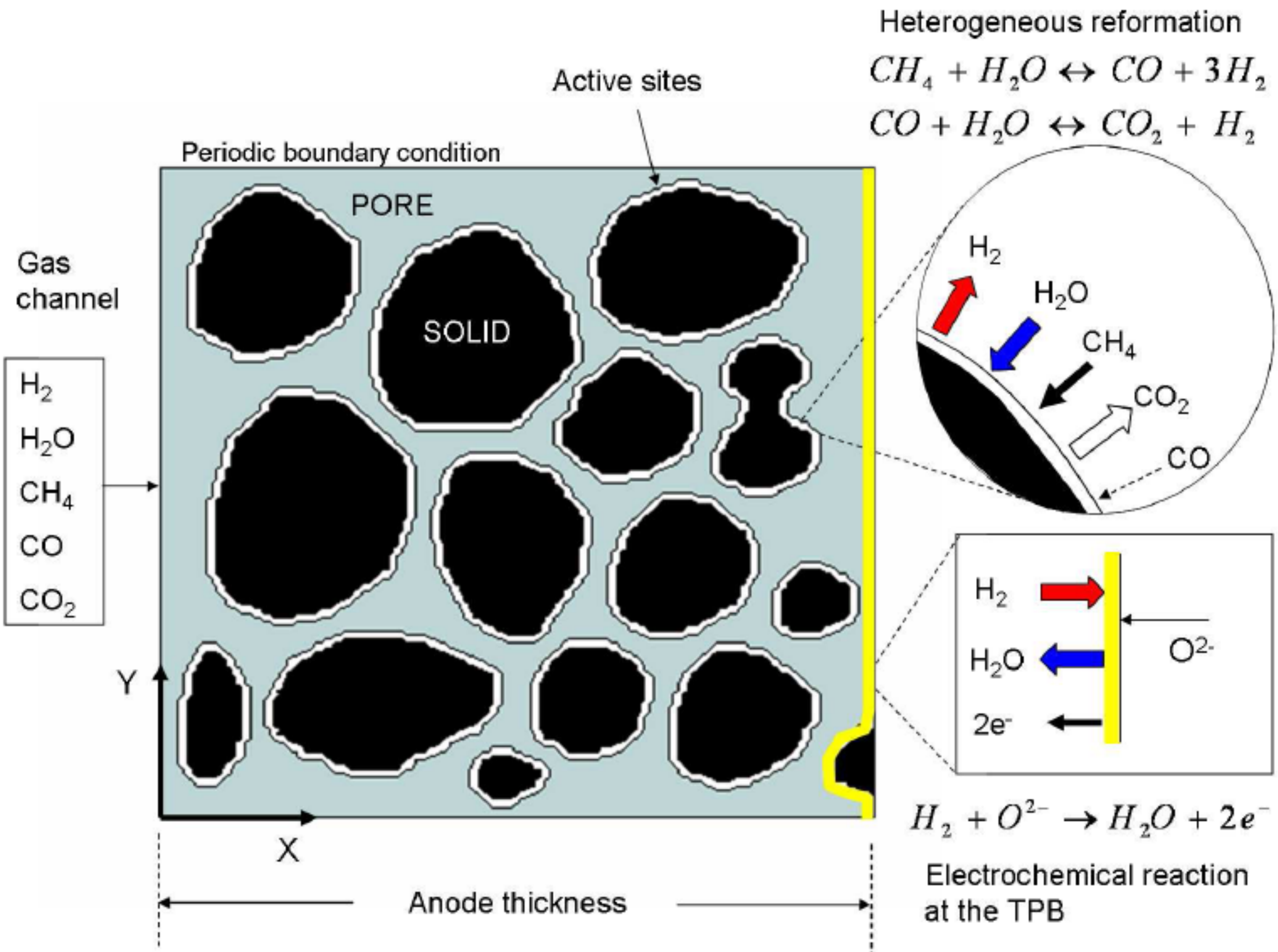




Validation with Previous SOFC Models



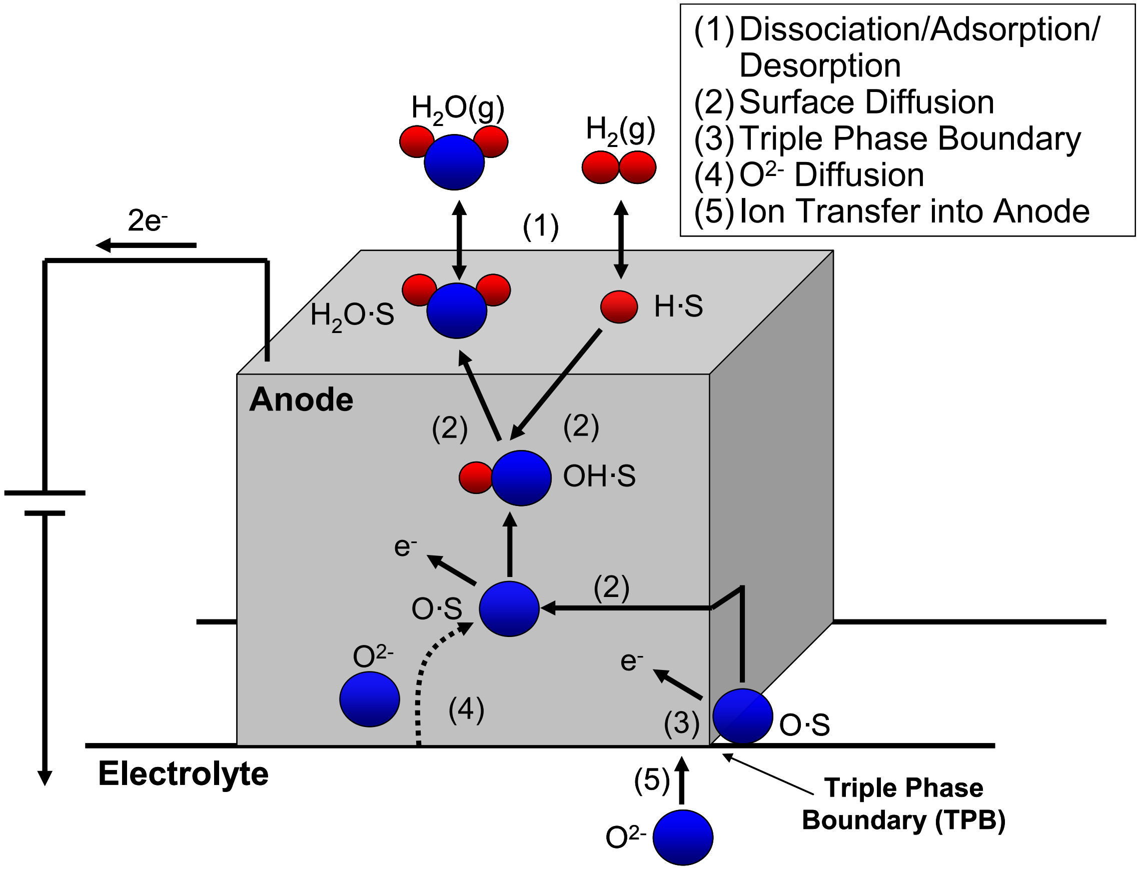
Coupled LBM + Reforming + Electrochemistry



Electrochemical Reaction Kinetics at the TPB

Global Reaction: $H_2^g + O^{2-}_{electrolyte} \rightarrow H_2O^g + 2e^-_{Ni}$

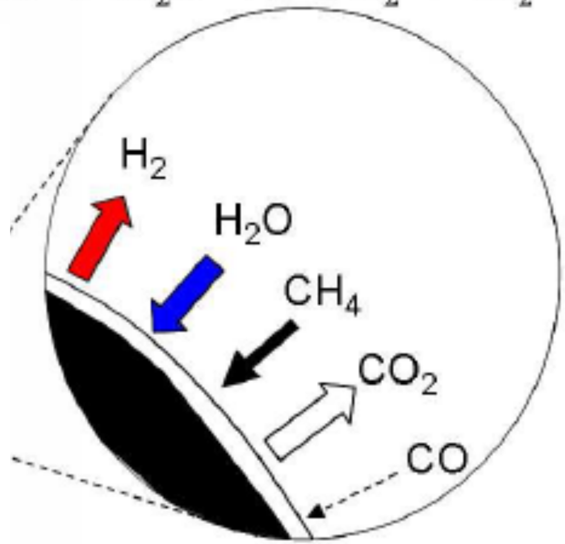
Reaction Mechanism *



* A. Bieberle and L.J. Gauckler, *Solid State Ionics*. **146:** 23-41, 2002.

Heterogeneous Reforming Reactions at Active Sites

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$
$$CO + H_2O \leftrightarrow CO_2 + H_2$$



- Detailed 40 step mechanism outlined by Zhu et al. (2005)*
- Provides flux boundary conditions for LBM gas transport model
- Flux is a function of the local species mole fractions

* H. Zhu, R. J. Kee, V. M. Janardhanan, O. Deutschmann and D. G. Goodwin, J. Electrochem. Soc. **152** (2005) A2427

Conclusions

- LBM is well-suited for modeling mass transport inside the SOFC anode.
- The LBM algorithm can be implemented efficiently on a parallel computer.
- LBM predictions for SOFC concentration polarization compare well with prior studies.
- The basic methodology can be extended to three dimensions, multiple components and coupled to separate models for electrochemical reactions / surface reforming reactions.
- This tool can help in analysis, design and optimization of SOFC.
- Applications for PEM fuel cells

Published Articles

1. Joshi A. S., Grew K. N., Peracchio A. A. and Chiu W. K. S. (2007) Lattice Boltzmann Modeling of 2D Gas Transport in a Solid Oxide Fuel Cell Anode, *Journal of Power Sources, 164, 631 – 638.*
2. Joshi, A. S., Peracchio, A. A., Grew, K. N. and Chiu, W. K. S. (2007) Lattice Boltzmann Method for Continuum, Multi-Component Mass Diffusion in Complex Geometries", *Journal of Physics D: Applied Physics, 40, 2961 – 2971.*
3. Joshi, A. S., Peracchio, A. A., Grew, K. N. and Chiu, W. K. S. (2007) Lattice Boltzmann Modeling of Non-Continuum, Multi-Component Gas Transport", *Journal of Physics D: Applied Physics, 40, 7593 – 7600.*

Coming Soon

4. Joshi, A. S., Izzo J. R. Jr., Grew, K. N., Peracchio, A. A. and Chiu, W. K. S. "Lattice Boltzmann Modeling of Three Dimensional, Multi-Component Mass Diffusion in a Solid Oxide Fuel Cell Anode", <u>submitted to</u> *Journal of Fuel Cell Science and Technology.*
5. Izzo J. R. Jr., Joshi, A. S., Grew, K. N., Chiu, W. K. S., Tkachuk, A., Wang, S. and Yun, W. "Structural Characterization of Porous Solid Oxide Fuel Cell Anodes using X-ray Computed Tomography at 50 nm Resolution" <u>submitted to</u> *Journal of the Electrochemical Society.*
6. Chiu, W. K. S., Joshi, A. S. and Grew, K. N. "Lattice Boltzmann method for Multi-component Mass Transfer in a Solid Oxide Fuel Cell Anode with Heterogeneous Internal Reforming and Electrochemistry" <u>submitted to</u> *European Physics Journal: Special Topics (Keynote presentation at the DSFD conference held in Banff, Canada, July 2007).*

Acknowledgments

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