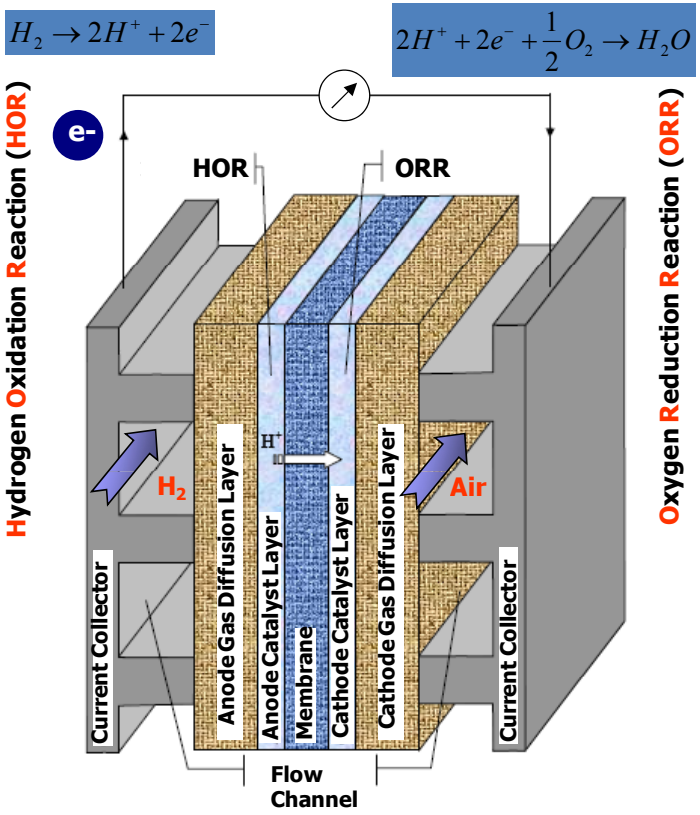
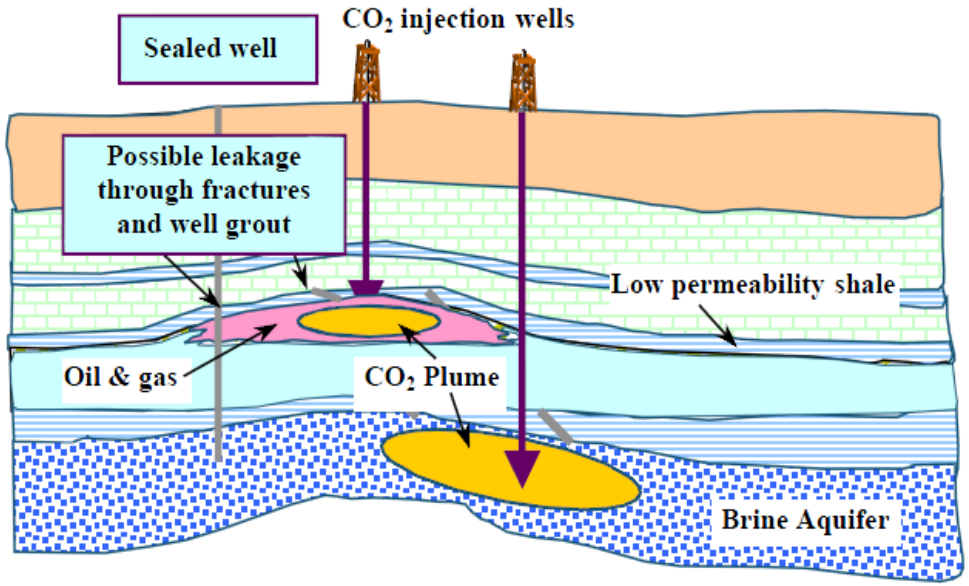
Multi-Physicochemical Transport/Interfacial Processes in Permeable Media

Multi-physicochemical transport/interfacial processes in natural/man-made permeable media are pervasive in energy and Earth systems



Hydrogen polymer electrolyte fuel cells



Geological CO_2 sequestration

Multi-Physicochemical Transport/Interfacial Processes in Permeable Media

Opportunity

A better understanding of these processes will have significant applications in a broad spectrum of energy and Earth research, including hydrocarbon production, development of geothermal reservoirs, geological storage of CO_2 and nuclear wastes, as well as engineered energy systems (fuel cells, batteries, micro power plants)

Meso Challenge

- **Current efforts in energy devices focus on nanoscale effects alone, lacking the foundations for an optimum mesostructural architecture to allow for efficient electrochemical activity**
- **There is a fundamental discrepancy in scales between the mesoscale where geochemical and microbiological reactions occur and the continuum scale where these processes are usually modeled.**

Approach

- **High performance computation based on mesoscopic approaches will expand our understanding of these processes**
- **The lattice Boltzmann method (LBM) is a mesocopic method occupying the middle ground between the micro and macro scales**
- **Taxila LBM, an open source, massively parallel software package developed in an ongoing LANL LDRD-DR project will be fully leveraged**

Impact

- **LBM mescoscopic modeling can help design optimal electrode structures and guide materials synthesis towards appropriate dimensions and functionality**
- **LBM modeling can bridge the gap between the pore (meso) and continuum (macro) scales and help resolve the scale dependence of reactive transport in the subsurface**

1. Q. Kang, P. C. Lichtner, D. R. Janecky, Lattice Boltzmann method for reacting flows in porous media, *Adv. App. Math. Mech.*, **2**, 545, 2010.
2. P. P. Mukherjee, Q. Kang, and C. Y. Wang, Pore-Scale Modeling of Two-Phase Transport in Polymer Electrolyte Fuel Cells - Progress and Perspective, *Energy Environ. Sci.*, **4**, 346, 2011.
3. https://software.lanl.gov/taxila/trac

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