

Abstract Submitted
for the DFD13 Meeting of
The American Physical Society

Simulation of water splitting reaction in porous media using Random Walk particle tracking method NIMA RAHMATIAN, University of Florida, JÖRG PETRASCH, Vorarlberg University of Applied Sciences, RENWEI MEI, JAMES KLAUSNER, University of Florida — Water splitting using iron-based looping process is a well-known method to produce high purity hydrogen. A stable porous structure is best suited for the reaction over many cycles due to high surface area. In order to simulate the reacting flow in the porous structure Random Walk method is used due to its ability to handle stiff reaction kinetics and varying hydrodynamic dispersion tensor caused by pore-level velocity fluctuations. Because of significant variation in bulk density during conversion of steam to hydrogen, Random Walk formulation needs to be modified to account for bulk density variations and source term due to chemical reaction. The species transport equation is recast in the form of Fokker-Planck equation and the trajectories of fluid particles are obtained by solving an appropriate Langevin equation that has additional drift terms due to spatial variations in bulk density and dispersion tensor. The source term is accounted for by changing the number or the composition of fluid particles based on the reaction kinetics. The treatment for each new term is validated using highly resolved finite difference solution. A bench-scale reactor for hydrogen production is simulated and excellent agreement with the measured hydrogen production rate is obtained.

Nima Rahmatian
Univeristy of Florida

Date submitted: 01 Aug 2013

Electronic form version 1.4