Virtual reality simulations of void structure, and absolute and relative permeability, in nano- to macro-scale materials, including nuclear reactor graphite and tight-oil shale

G. Peter Matthews

University of Plymouth and PoreXpert Ltd, UK

The inverse modelling of percolation measurements of porous materials (mercury porosimetry, porometry or soil water retention) can yield realistic void structure simulations, provided that void clusters are taken into account. We have studied porous materials with voids spanning sizes from nanoporous (1nm) to macroporous (100 microns), specifically nuclear reactor graphite and tight-oil shale. The behavior of pore fluids within the voids depends on the concerted action of all the voids over the entire size range, so that traditional 'hierarchical' and 'dual pore' models are inappropriate. We present fully integrated void structures in 3D virtual reality for nuclear reactor graphite (Gilsocarbon) and tight-oil shale, represented as infinitely repeating 'unit cells', with each unit cell comprising around 44000 void features. Of particular importance, both in Advanced Gas-cooled nuclear Reactors (AGRs) and in tight-oil reservoirs undergoing hydraulic fracturing, are the absolute and relative permeabilities respectively. We demonstrate how the application of multiple Navier-Stokes equations across the void networks gives realistic estimates of these permeabilities, which are difficult or impossible to measure in a laboratory. Uniquely, for tight-oil shale, the inverse modeler (PoreXpert) can be used to simulate the effect on relative permeabilities of wettability differences to oil and brine, and changing flow velocities during huff-puff extractions. Many other pore-fluid simulations are possible, such as dynamic wetting, and depth filtration effects occurring during the application of colloidal suspensions. Simulations can also be made of changes to the void structure induced by, for example, weathering and hydraulic fracturing.

Biography

Peter Matthews trained at Oxford University, and was subsequently awarded a college lectureship at St Catherine's College. He is Emeritus Professor of Applied Physical Chemistry at the University of Plymouth, UK, and a Director and CEO of its spin-out company PoreXpert Ltd. He is also a member of the EDF Energy Independent Graphite Validation Group advising on active core weight loss, and consequent end-of-life, of the U.K's fleet of AGR nuclear reactors. During his career at Plymouth University, he attracted £4.5m of research funding, and published 100 research publications and a textbook on Experimental Physical Chemistry (Oxford University Press).