Research Interests and Accomplishments

My work on modeling of transport phenomena in porous media [6, 7] has involved study of concurrent transport processes that are nonlinearly coupled to each other, to changes in the properties of the medium, or to chemical reactions. Examples include diffusion of chloride into concrete [4], flows of compressible fluids through compressible porous media [3, 5] (relevant to analysis of hydraulic transients in water and oil/gas reservoirs), advective transport with concurrent adsorption [2] (relevant to groundwater pollution, design of novel materials for chromatographic separations and gas purification/storage), CO_2-enhanced coalbed methane recovery, and electrodeposition of porous insulating layers [1, 45, 46] (relevant to the corrosion protection of metals and the behavior of porous battery electrodes.) Additional nonlinearities can also result from interfacial conditions, as in diffusion of hydrogen through layered composites [9, 10, 11, 12, 13, 14].

Since the chemical potential gradient is the driving force for material transport, deviations from thermodynamic ideality in general correspond to nonlinear transport behavior. Thermodynamic study of electrolyte solutions under conditions where pronounced nonidealities are expected (found in geothermal fields and the steam cycles of power plants) was the focus of my work in the high-temperature aqueous chemistry group at ORNL [17,27,30-35] and in an earlier appointment at Murdoch University [43,44].

As a result of my original training in experimental physical chemistry [68], collaboration with experimentalists has been an important theme in my research, in the design of equipment [19,28,42,56] and analysis of results [20,23-25]. In connexion with the development of errors-in-variables methods for parameterization of nonlinear thermodynamic models [15,21,22], I acquired experience in the use of a variety of optimization techniques.

My interest in applied mathematics developed not only from my doctoral [61-67] and subsequent work [49-52] on theoretical electrochemistry, but also from applied research at ANL. In addition to experimental work [48,57-60], I developed an interest in the calculation of current distributions in electrochemical cells with resistive [39,41,47,53] and porous [54,55] electrodes. Work on accelerating the convergence of the Fourier series arising in these applications [37,38] led to development of rapidly convergent Green functions for the Laplace/Poisson equation with Neumann [36] or periodic [26,29] boundary conditions. The periodic Green functions are relevant to molecular dynamic simulation of polar fluids, and to solid-state electronic structure calculations.

List of Publications

[1] Simon L. Marshall. Ionic diffusion and migration fluxes in passive film formation under mixed kinetic control. In F. Chan, D. Marinova, and R.S. Anderssen, editors, *Proceedings of the 19th International Conference on Modelling and Simulation*, pages 324–330. Modelling and Simulation Society of Australia and New Zealand, Perth, Western Australia, December 12-16 2011.

[2] Simon L. Marshall. Concurrent diffusion and adsorption in nanoporous materials. In D. Bhattacharyya, R.J.T. Lin, and T.S. Srivatsan, editors, *Proceedings of the 19th International Conference on Processing and Fabrication of Advanced Materials*, pages 771–784. Auckland, New Zealand, January 14-17 2011.

[3] Simon L. Marshall and Raj Das. Medium- and fluid-compressibility effects in flows through hot sedimentary aquifers. In G.D. Mallinson and J.E. Cater, editors, *Proceedings of the 17th Australasian Fluid Mechanics Conference*, pages 169–172. Auckland, New Zealand, December 5-9 2010.

[4] Simon L. Marshall. Chloride penetration into concrete with time dependent diffusivity and boundary concentration. To be submitted for publication in *Cement and Concrete Research*. Approved for publication.

[5] Simon L. Marshall. Nonlinear pressure diffusion in flow of compressible liquids through porous media. *Transport in Porous Media*, 77(3):431 – 446, 2009.

[6] Simon L. Marshall. Mathematical analysis of diffusive processes in porous media. Technical Report 08/125, CSIRO Mathematical and Information Sciences, 2008. This report presents an overview of the analytical techniques that have been applied to the analysis of diffusive transport phenomena in porous media.

[7] Simon L. Marshall. Molecular modelling in meso-scale systems: an annotated bibliography. Technical Report 08/12, CSIRO Mathematical and Information Sciences, 2008.

[8] Simon L. Marshall. Fundamental aspects of microbial enhanced oil recovery: a literature survey. Science report series, CSIRO Land and

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