Modelling of Solid Oxide Fuel Cells

Fuel cell technology is a rapidly expanding field and high temperature (~900 °C) SOFCs are likely to play an important role in medium-sized power generation systems from 2010 onwards, see the review [2007]. In particular, the combination of SOFC and gas turbine holds the promise of very high cycle efficiency coupled with ultra-low pollutant emissions. Rolls-Royce Fuel Cell Systems Ltd are currently developing a MW-scale SOFC-GT system and Cambridge is involved in both theoretical analysis and development of computational techniques. Modelling work is challenging because it is necessary to address so many different physical phenomena. These include the electrochemical reactions, multi-component diffusion in the porous parts of the structure, surface-catalysed chemical reactions, heat transfer in the gas flows and solid structures, and the electric current distribution.

Several papers have now been published on different aspects of this work [2002, 2004a, 2005a]. The most ambitious calculation to-date is a fully three-dimensional simulation of the multi-component reactive-diffusive flows in the fuel cell and reforming stacks, which allows simulation of all the important physical and chemical processes in an internal double-module of the Rolls-Royce design [2004b, 2006, 2008]. This computer code is one of the most advanced SOFC simulator of its type in the world at present.

The SOFC modelling work has also led to a most interesting re-assessment of multi-component convection-diffusion in porous solids at arbitrary Knudsen number [2005b]. This analysis provides physical insight, new theoretical results and an improved method of interpreting experimental data, all of which should also be of interest to the chemical engineering, as well as the fuel cell, community.

Low-speed internal flows at transition regime Knudsen numbers less than about 0.5 have sometimes been calculated using the Grad 13-moment (G13) method. Recently the ‘regularised’ 13-moment (R13) method with improved closure conditions has been proposed. An assessment of the R13 method has been made by applying it to the classical problems of velocity slip, temperature jump and thermal creep [2011]. It turns out that although the Knudsen layer associated with thermal creep is well-represented by the R13 theory, the layers associated with velocity slip and temperature jump are not.

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