

COMPUTATIONAL FLUID DYNAMICS STUDIES OF FUEL CELLS

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ABSTRACT

Physicochemical hydrodynamics may be considered as an inter-disciplinary science which deals with the effects of fluid mechanics on physical and chemical processes, and vice versa. The subject was pioneered by Prof. D.B. Spalding and his friend and colleague V.G. Levich. Fuel cells are electrochemical devices which convert chemical energy to useful electricity, and waste heat. Starting with Prof. Spalding's PHOENICS code in 1999, the present author and his associates have been building models of fuel cells at the sub-cell (micro-scale), cell, and stack levels up to the present day. These include models of high-temperature solid oxide fuel cells, where thermal radiation is significant, and also low/medium temperature polymer electrolyte technologies suitable for non-stationary applications. Large stacks are modelled using a 'distributed resistance analogy', originally proposed by Patankar and Spalding for heat exchanger design studies, and modified by introducing Spalding's ground-breaking approach to mass transfer. Micro-scale models are used to compute effective transport properties, difficult to obtain experimentally, for utilisation in cell-level models. This idea, also, was originally suggested by Spalding in the context of heat exchanger analysis. Cell-level calculations for fuel cells, may include single-phase or multi-phase flow in the gas channels, porous diffusion, active catalyst, and ionically-conducting membrane-electrolyte layers, as well as heat/mass transfer, chemical and electrochemical kinetics. For multi-phase flow; liquid-gas phase-change, surface-tension, and gas solubility are all important factors that require to be taken into consideration. Currently our fuel cell codes employ 10-100 million computational mesh cells, and run efficiently on large parallel computing facilities.