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Modeling and Simulation of Power Yield in Chemical and Electrochemical Systems

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Abstract. Fuel cells are treated as flow engines driven by fluxes of chemical reagents and electrochemical mechanism of electric current generation. Analyzed are performance curves of a SOFC system, power limits and the effect of typical design and operating parameters on the cell performance. The theory combines a recent formalism worked out for chemical machines with the Faraday's law which determines the intensity of the electric current generation. Steady-state model of a high-temperature SOFC is considered, which refers to constant chemical potentials of incoming hydrogen fuel and oxidant. Lowering of the cell voltage below its reversible value is attributed to polarizations and imperfect conversions of reactions. A power formula summarizes effect of transport laws, irreversible polarizations and efficiency of power yield. Reversible electrochemical theory is extended to the case with dissipative chemical reactions; this case includes systems with incomplete conversions, characterized by "reduced affinities" and an idle run voltage. Effect of incomplete conversions is modeled by assuming that substrates can be remained after the reaction and that side reactions may occur. Optimum and feasibility conditions are discussed for some important process parameters such as the efficiency, power output, and electric current density. Calculations of maximum power show that the data differ for power generated and consumed. These data provide bounds for SOFC energy generators, which are more exact and informative than classical reversible bounds for electrochemical transformation.

Key words

Power limits, entropy, chemical engines, fuel cells.

1. Introduction

In a previous work [1] we modelled power production and its limits in purely thermal systems with finite rates. In particular, radiation engines were analyzed as nonlinear systems governed by laws of thermodynamics and transport. Temperatures T of resource media were only necessary variables to describe these systems. However, chemical engines and fuel cells are more general systems in which both temperatures T and chemical potentials μ_k are essential. A chemical engine is schematized in Fig. 1, whereas a solid oxide fuel cell SOFC in Fig.2. Fuel cells (FC) are electrochemical flow engines. Their role for environmental protection cannot be underestimated. The main advantage of fuel cells in comparison to heat engines is that their efficiency is not a major function of device size.

A fuel cell continuously transforms a part of chemical energy into electrical energy by consuming fuel and oxidant. Fuel cells are electrochemical flow engines propelled by fluxes of both energy and substances.

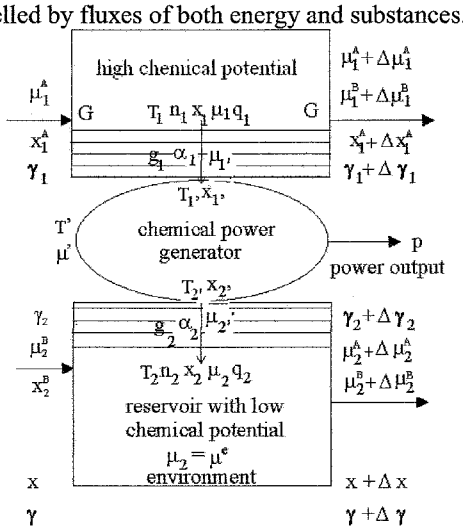

Fig.1. A scheme of chemical flow engine.

The symbols in Fig. 1 describe: μ - chemical potential of active component of fuel [Jmol^{-1}], γ-cumulative conductance of the system [Js^{-1}K^{-a}], x - molar fraction of active component in the fuel, T_1 and T_2 - bulk temperatures of reservoirs [K], $T_{1'}$ and $T_{2'}$ - temperatures of fluid circulating in the engine [K], T^e - constant temperature of environment [K], T' - Carnot temperature [K], α - heat coefficient [Jm^{-2}s^{-1}K^{-1}], q - heat flux [Js^{-1}], g_1 and g - partial and overall conductances [mols^{-1}]).

Basic structure of fuel cells includes electrolyte layer in contact with a porous anode and cathode on either side. Gaseous fuels are fed continuously to the anode (negative electrode) compartment and an oxidant (i.e., oxygen from air) is fed continuously to the cathode (positive electrode) compartment. Electrochemical reactions take place at the electrodes to produce an electric current. Basic reaction is