Description of the software "SINGLE-CHAMBER SOFC PROCESS MODELLING"

The software is designed to simulate the processes in the physical vapour deposition of the fuel cell solid electrolyte and electrodes, as well as the kinetic mass transfer and catalytic processes in single-chamber solid oxide fuel cells (SINGLE-CHAMBER SOFC). It consists of three parts describing oxygen diffusion, thin film growth modelling, and the influence of internal stresses on the ion transfer process. To start the programme, select a file "OPEN program", then:

1. To calculate the distribution of oxygen ions in the electrolyte of a single-chamber solid-state fuel cell when chemical reactions take place on the cathode and anode sides during oxygen ion transfer, select the "Fuel cell - Oxygen diffusion MODEL".

Input parameters: By using two separate 2D matrices of anode and cathode distribution that should be kept on the desktop, it is possible to change the given computational conditions as the sizes of the smallest element of the electrolyte dx, dy, dz, the number of elements forming the electrolyte in the x, y, z directions. In order to proceed to simulation, the reaction rate constants ki, gas composition and pressure must be entered.

Output: After simulation, 3D sections of the electrolyte are obtained and the oxygen ion concentration distribution is observed. In addition, the programme simulates the oxygen ion flux on both the cathode COKJ and anode COAJ sides with respect to time and determines the total oxygen ion concentration in the COt electrolyte with time.

2. To model the growth kinetics of thin films formed by physical vapour deposition, select the "Phase structure MODEL".

Input parameters: Growth time of the thin film; time step of the simulation experiment; magnitudes of the computational grid in the x, y, z directions; values of the adhesion coefficients k_{AA}, k_{AB}, k_{AS}, k_{BA}, k_{BB}, k_{BS}; the proportionality coefficient p_A; the proportionality coefficient p_B; the coefficient γ (energy 'gradient'); the parameter of the polynomial function of the free energy of the homogeneous system; the positions of the planes over which the cross-sectional images are drawn.

Output: By clicking the "Calculate" button starts the thin film growth simulation experiment (using the parameter values in the text boxes). When any calculation is completed, the programme saves all the final calculation data in the "Results.txt" document in the programme directory and plots the cross-sectional images over the planes specified at the time. By clicking on the "Draw cross-sectional images" button, it is possible to redraw the cross-sectional images in any of the planes perpendicular to the x, y, z axes.

3. To calculate the variation of the oxygen ion concentration in the electrolyte of a single-chamber solid-state fuel cell by taking into account the internal stresses due to the diffusion of oxygen ions and their influence on the ion transport process, the "Stress and diffusion MODEL" must be selected.

Input parameters: diffusion process duration; process temperature; relative oxygen ion flux; diffusion coefficient; diffusion activation energy; stress characterisation factor.

Output: Pressing the "START" button starts the simulation experiment of the oxygen ion transfer process (using the parameter values in the text boxes). After any calculation is completed, the profiles of the oxygen ion concentration distribution and internal stresses are displayed in the programme window.