Modeling of hydrogen gas driven permeation through membranes

A. Pisarev*, I. Tsvetkov, S. Yarko, and E. Marenkov

National Research Nuclear University (MEPHI), Kashirskoe sh. 31, Moscow 115409, Russia

Features of gas driven permeation through membranes in transition and steady state regimes obtained by modelling of the permeation are outlined. The diffusion equation and boundary conditions including the second order desorption are used. Steady state permeation through asymmetric membranes is considered; the permeation is characterized by introducing two transport parameters; the cases of diffusion limited regime (DLR) and surface limited regime (SLR) are characterised; boundaries and approximations for the two regimes are given. Time dependencies of permeation through asymmetric membranes in two regimes are compared, and validity of analytical approximations in intermediate regimes is analysed. Multilayer membranes are considered; analytical solutions for DLR and SLR transient permeation rates are given; steady state permeation equations for concentrations and permeation fluxes are obtained and analysed; features of temperature dependencies and sequence of layers are discussed. Transition from the multilayer membrane to the membrane with continuously changing properties is performed. Influence of traps and validity of the effective diffusion coefficient approach is analysed; contradictions in description of the concentration profiles and permeation rates are demonstrated. Influence of pores on permeation is touched with emphases on hydrogen gas accumulation in pores; effects of point defects and that of pores are compared. Three dimensional numerical modelling of permeation through membranes with rough surface is performed; influence of roughness on the two sides of the membrane in various regimes is analysed. Three dimensional modelling of permeation through protection layers with cracks is performed; and decrease of the efficiency of the protection barrier due to its imperfection is analysed in various regimes.