Numerical analysis of species diffusion and methanol decomposition in thermocatalytic reactor based on the intermetallic phase of ni𝟑al for low reynolds numbers

Ziokowski, Pavel, author

Abstrak

Numerical modelling of hydrogen production by means of methanol decomposition in a thermocatalytic reactor using corrugated foil made of the Ni3Al intermetallic phase is shown in the paper. Experimental results of the flow analysis of mixtures containing helium and methanol in a thermocatalytic reactor with microchannels were used for the initial calibration of the CFD calculations (calculations based on the Computational Fluid Dynamics method). The reaction of the thermocatalytic methanol decomposition was modelled based on experimental data, considering the size of the active surface. The drop in the methanol concentration at the inlet to the reactor, ten millimetres in front of the thermocatalytic region, is associated with the diffusion of streams of other components, mainly hydrogen and carbon monoxide. The commercial CFD code was expanded by User Defined Functions (UDFs) to include surface chemical reaction rates in the interphase between the fluid and the solid. Extrapolation of data by means of the implemented numerical model enabled the assessment of the minimum length of microreactor channels and prediction of the optimal dimension at the system outlet. The results obtained by means of numerical calculations were calibrated and compared with the experimental data, confirming a satisfactory consistency of the data