MODELING OF HEAT AND MASS TRANSFER PROCESSES IN METAL HYDRIDE REACTOR

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Reaction and equilibrium properties of metal hydrides systems AB_2 and AB_5 based on lanthanum and zirconium alloys are investigated. Equilibrium properties are presented in analytical form using Vant Hoff's equation and De Bur's relationship validated for system with complicated phase composition. It is shown that for *La* alloys family $La_{1-X}Ni_{5-Y}Ce_XAl_Y$ variation of their content from $Y = 0$, $X = 1$ to $Y = 0$, $X = 0$ increases equilibrium pressure up to 3-4 orders of magnitude, while for $Zr_{0,9}Ti_{0,1}Cr_{1-Y}Fe_{1+Y}$ alloys family it increases up to one order at Y varying from 1 to 1.4. Analytical solution describing charging-discharging dynamics of metal hydride reactor, destined for accumulation of hydrogen and operating either at constant pressure or constant hydrogen flow rate, is presented.

The solution is confirmed by experimental results of hydrogen accumulator study at heat carrier temperatures varying in range of 20 – 90 °C and pressures in range of 5 – 20 atm. Modeling of pair metal hydride reactors, realizing heat pump cycle, is fulfilled, using the mathematical solution. Optimization of heat energy output at the given thermal resources of the source and sink of heat and the required temperature of recovered heat source is demonstrated through the choice of the proper metal hydride pair inside of the investigated range of compositions.