ABSTRACT

The world is witnessing an inevitable shift of energy dependency from fossil fuels to cleaner energy sources like wind, solar, hydrogen, etc. The governments from all over the world have realized that for limiting the global rise in temperature to 1.5 °C, hydrogen has to be given a reasonable/sizable share in meeting global energy demand by mid of 20^{th} century. Hydrogen can be produced through several means using renewable energy sources and can be stored either in solid, liquid or gaseous state. Though, compressed and liquefied hydrogen storages are well-established technologies in the commercial sector, however, due to the leakage risk, boil-off losses and explosive nature, world is exploring a safer way of hydrogen storage i.e. absorption/adsorption based solid-state hydrogen storage technology. Although hydrogen can be produced from various extraction processes, such as through decomposition of fossil fuels, electrolysis of water, thermolysis of water, biomass conversion, etc., it is not always in the pure form. Metal hydride (MH)- hydrogen system can be a suitable solution for safe hydrogen storage and easy purification technology. Considering these issues, in the present study, thermodynamic screening of MH alloys was studied to filter suitable alloys for efficient working of metal hydride based hydrogen purification system MHHPS. From alloy screening, $LaNi_{4.7}Al_{0.3}$, $LaNi_5$ and $La_{0.9}Ce_{0.1}Ni_5$ alloys were considered for MHHPS. In order to check feasibility of metal hydride (MH) for hydrogen storage and purification application, parametric investigation of $LaNi_{4.7}Al_{0.3}$, $LaNi_5$ and $La_{0.9}Ce_{0.1}Ni_5$ alloys have been performed by varying different set of experimental parameters like hydrogen supply pressure, absorption temperature, and desorption temperature at fixed flow rate of 'heat transfer fluid (HTF)' at 4 lpm. The experiments have been carried out using 6 ECT reactor configuration. The rector was designed using numerical simulations performed using COMSOL Multiphysics, and further the numerical results were validated using experimental data. The results show that, all the selected alloys were suitable for hydrogen storage and purification application. Parametric studies for optimizing the operational parameters of the coupled reactor in multi-stage MHHPS were performed. For efficient system operation, the suggested absorption temperature is in the range of 20 °C to 30 °C with supply pressure 5 bar to 20 bar, while the flushing and desorption are suggested in the ranges of 15 °C to 20 °C and 70 °C to 90 °C, respectively. Further, for TCD (thermal conductivity detector) analysis, an optimum method has been developed for GC (gas chromatography), wherein column flow is fixed at 6 mL/min and oven temperature is raised from 60 °C to 150 °C. The system was calibrated with standard gas sample. The poisoning effect of various gaseous impurities (mainly CH_4, CO_2, CO, N_2, Ar) in the single and

multi-stage MHHPS has been investigated by varying the impurity level from 10% to 50% by weight in H_2 gas mixture and by performing cyclic test with 10% impurity level. The system includes a reactor configured with embedded cooling tubes, centrally located SS316 sintered porous filter, an identical three bed space, each filled with 1.2 kg $La_{0.9}Ce_{0.1}Ni_5$, $LaNi_5$ and $LaNi_{4.7}Al_{0.3}$ alloy, a cold and hot fluid supply line with a fluid pump, and gas valves. According to the results, the system delivered 100% pure hydrogen for 10% to 20% impure gas mixture in a single stage. While, for higher impurity level, the purity level of desorbed hydrogen was in the range of 95% to 99.9% for single stage operation. However, for higher impurity, the multistage operation is capable to deliver pure hydrogen (99.9995%). According to the cyclic study, the reaction kinetics of the reactor bed got affected significantly. The poisoning effect of gases are in the order $Ar<N_2<CH_4<CO_2<CO$. Moreover, it is not suggested to use CO above 0.5-1%. Further, for large scale hydrogen storage and purification, 99 ECT reactor was filled with 40 kg $LaNi_{4.7}Al_{0.3}$, having hydrogen storage and purification capacity of over 6000 l, in a single stage.