INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **DESIGN AND PERFORMANCE ASSESSMENT OF MULTISTAGE METAL HYDRIDE HYDROGEN COMPRESSORS**

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SHORT ABSTRACT

This thesis addresses a critical gap in the advancement of metal hydride-based hydrogen compressors (MHHCs) capable of delivering hydrogen at pressures exceeding 250 bar while operating under a temperature limit of 100 °C. To this end, a three-stage MHHC was systematically designed, developed, and experimentally validated. The alloys $La_{0.8}Ce_{0.2}Ni_5$, $La_{0.3}Ce_{0.7}Ni_4Fe$, and $Ti_{0.8}Zr_{0.2}CrMn_{0.3}Fe_{0.6}Ni_{0.1}$ were strategically selected for the primary, intermediate, and final stages, respectively, based on their Pressure–Composition–Temperature (PCT) characteristics. A comprehensive multiphysics mathematical model was developed in COMSOL, incorporating key hydride-specific features such as hysteresis, slope factor, and lattice volume expansion. This model served as an effective design and optimisation tool for high-pressure reactor geometries and system-level performance. Guided by model insights, two modular reactors each comprising 19 alloy-filled high-pressure tubes, were fabricated to house 50 kg of alloy per stage, enabling the compression of over 6200 L of hydrogen per stage. Six such reactors, integrated with custom-engineered heat transfer fluid (HTF) circuits and a dedicated gas handling manifold, constitute the industrial-scale MHHC system developed in this work, which is currently operational at NTPC NETRA. Activation studies confirmed that complete activation of all three alloys was achieved within 4–8 cycles. Performance evaluation of $Ti_{0.8}Zr_{0.2}CrMn_{0.3}Fe_{0.6}Ni_{0.1}$ demonstrated that an injection pressure of 100 bar enhanced absorption kinetics by a factor of 2.5, achieving a system-level gravimetric storage capacity of 0.55 wt% and delivering 210 bar hydrogen at 50 °C, with a gravimetric exergy recovery of 14.8 W/kgMH. Parametric studies on $La_{0.3}Ce_{0.7}Ni_4Fe$ revealed an optimal injection pressure of 40–50 bar with HTF at 10 °C, while complete desorption occurred only above 60 °C. Similarly, $La_{0.8}Ce_{0.2}Ni_5$ exhibited strong absorption at 15 bar with HTF at 15 °C, but required a minimum of 70 °C for full desorption. A dual-stage prototype system, employing $La_{0.3}Ce_{0.7}Ni_4Fe$ in the first stage and $Ti_{0.8}Zr_{0.2}CrMn_{0.3}Fe_{0.6}Ni_{0.1}$ in the second, successfully compressed 500 NL of hydrogen from 40–50 bar to 313 bar within a 5–80 °C operating window. To extend hydrogen intake capability down to 15 bar, the industrial-scale system incorporated $La_{0.8}Ce_{0.2}Ni_5$ as the primary stage. The fully integrated MHHC demonstrated reliable hydrogen compression from 15 bar to 300 bar over 5–91.2 °C. The standalone first-law efficiency ranged between 5–8%, while integration with waste heat recovery boosted the overall system efficiency to 46.25%.