Studies on Catalytic Decomposition of Hydrogen Iodide in Sulphur-Iodine Cycle for Hydrogen Production

Abstract

Nowadays, increasing global energy demand, fossil fuel dependence for energy generation, and resulting CO₂ emissions multiply economic and environmental concerns. On the other hand, hydrogen is a clean energy carrier that can eliminate greenhouse gas emissions and meet future energy needs. Sulfur-Iodine (SI) thermochemical cycle is a highly efficient, eco-friendly, and lower temperature (~900°C) water-splitting process for hydrogen production. There are three main reactions in the cycle: Bunsen, sulphuric-acid decomposition, and hydrogen iodide (HI) decomposition. HI decomposition is an essential step of this cycle because hydrogen is formed here. It is an endothermic, reversible, and equilibrium-limiting reaction. There is no remarkable conversion of HI without the catalyst, even at 550°C. The literature primarily focussed on Ptbased catalysts and costly hydrogen-permeable membranes, which affect the overall cost of the cycle. Hence, there is a need for cost-effective, active, and stable catalysts and a feasible approach for attaining conversion above equilibrium in a fixed bed continuous flow reactor. In the present study, NiO-ZrO₂ in xerogel form was synthesized by a single-step epoxide-driven sol-gel method with different nickel content that showed HI conversion of 23.6% at 550°C. The catalyst (5 wt% NiO-ZrO₂) was tested with an adsorbent for iodine removal to increase the conversion above equilibrium. Activated Carbon (AC) was selected as an iodine adsorbent that potentially exhibited catalytic properties for HI decomposition reaction. The catalyst and adsorbent were arranged in different assemblies inside the reactor bed to find a suitable configuration. The intermixed assembly showed maximum conversion at 500°C, i.e., 25.6%, which was 2.6% above the equilibrium value. The catalyst and synthesized adsorbent (5 wt% iodine impregnated on AC) were investigated to confirm the role of adsorbed iodine in intermixed assembly at 500°C. It has been observed that a significant conversion of ~35% was achieved, indicating I₂/AC adsorbent triggered the conversion owing to its intervention that allowed the system to cross the equilibrium barrier. The long endurance test measured with catalyst and I_2/AC in the intermixed assembly at 500°C showed excellent stability of ~50 h. Thus, this increase in conversion beyond equilibrium through iodine removal in a packed bed continuous flow reactor is a practically feasible, stable, and economical approach.