Hydrogen High-Pressure Gas Storage in Type IV Tanks: A Molecular Simulation Study on Hydrogen Permeation in Polyamide 6 Liner Under Dry and Humid Conditions

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Enabling the widespread use of hydrogen as an energy carrier requires storage systems capable of achieving high volumetric densities—typically around 40 g/L—to ensure sufficient energy per unit volume. This requirement is most effectively met through high-pressure gas storage (up to 70 MPa), which has become the predominant method for onboard storage applications such as fuel cell vehicles. In this context, hydrogen storage technology has evolved toward Type IV tanks, which consist of a polymeric liner wrapped in a carbon fiber composite shell. These tanks offer key advantages over traditional all-metal counterparts, including reduced weight, embrittlement-free operation, and greater design flexibility. Polyamide 6 (PA6), a semicrystalline polymer, is widely employed as a liner material in Type IV tanks due to its favourable mechanical properties and intrinsic hydrogen barrier performance. However, PA6 is also highly hygroscopic, a characteristic known to influence its mechanical behaviour and expected to impact its gas transport properties. While the effects of moisture on mechanical performance are well established, the implications for hydrogen permeation remain largely unexplored, particularly under high-pressure conditions. This study investigates the influence of moisture on hydrogen transport in PA6 liners through a combination of Monte Carlo (MC) and Molecular Dynamics (MD) simulations. Hydrogen sorption, diffusion, and permeation were first modelled in the dry polymer up to 70 MPa, showing excellent agreement with available experimental data and validating the simulation approach. The investigation was then extended to simulate water uptake across a range of relative humidities, quantifying absorbed water and providing novel molecular-level insights into water–polymer interactions, clustering behaviour, and changes in polymer free volume. Finally, the ternary system involving hydrogen, water, and polymer was assessed to understand the impact of moisture on hydrogen transport properties—an area not previously studied, particularly due to the experimental challenges of characterizing high-pressure behaviour in humid environments. These findings support the design of advanced barrier polymers with improved performance in realistic service conditions, informing material selection and processing strategies for Type IV tank liners. Such developments are essential for enabling safe, lightweight, and efficient hydrogen storage systems that are critical to the transition toward a hydrogen-based economy.

Keywords: *Hydrogen Storage, Gas Transport in Polymers, Polymer Permeability, Molecular Simulations.*