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Simulation of cryo-adsorptive hydrogen storage performance of type III hydrogen storage tank in a wide pressure range

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Hydrogen is an important green energy source, but its low density and low boiling point bring problems for large-scale storage and transportation. Presently, liquid hydrogen storage and high-pressure gaseous hydrogen storage are two main hydrogen storage technologies. However, Liquid hydrogen storage has the problems of ortho-para hydrogen conversion and high liquefaction energy consumption; high-pressure gaseous hydrogen storage has a low hydrogen storage density which is only around 5 wt% at 70 MPa. Cryo-compressed hydrogen storage can effectively enhance hydrogen storage density, achieving liquid hydrogen density at 80 K and 48.52 MPa, but still faces issues of high hydrogen storage pressure and relatively high energy consumption. Adsorption-based hydrogen storage holds promise for improving current hydrogen storage technologies. For instance, MOF-210 exhibits a material-based gravimetric hydrogen storage density of 15 wt% at 77 K and 8 MPa. Combining porous adsorbent materials with cryo-compressed hydrogen storage for cryo-adsorptive hydrogen storage offers a new approach to achieve higher hydrogen storage density at relatively lower hydrogen storage pressures.

However, current researches on cryo-adsorptive hydrogen storage primarily focus on the synthesis of new porous materials and the measurement of their own hydrogen storage capabilities. The experiments and simulations predominantly concentrated in the low-pressure range (below 10 MPa). There is still a lack of research on low-temperature and high-pressure adsorptive hydrogen storage systems. Therefore, we establish a Type III hydrogen storage tank model by using finite element analysis software COMSOL Multiphysics. Activated carbon AX-21, metal-organic frameworks MOF-177, MOF-5, compacted MOF-5, Cu3(BTC)2 and MIL-101 are added to the Type III hydrogen storage tank, respectively. The modified Dubinin-Astakhov (D-A) model is used to simulate hydrogen adsorption isotherms, and the reliability of the model is validated. Subsequently, we simulate and predict the gravimetric/volumetric hydrogen storage density of the Type III hydrogen storage tank with different adsorbent materials at 77 K and pressures ranging from 1 to 50 MPa, and then study the effect of filling ratio on the overall gravimetric/volumetric hydrogen storage density.

The results show that at 77 K, activated carbon AX-21 and compacted MOF-5 achieve a gravimetric hydrogen storage density of 5.5 wt% at 41.4 MPa and 42.7 MPa, respectively, reaching the hydrogen storage target set by the U.S. Department of Energy for 2025. Additionally, compacted MOF-5 exhibits a volumetric hydrogen storage density comparable to liquid hydrogen at 77 K and 28.5 MPa, demonstrating excellent hydrogen storage performance and promising application prospects.

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