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Design of Functionally Graded Adsorption Beds for Gas Storage

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Abstract

Adsorption is the adhesion of molecules on surfaces due to van der Waals or covalent forces and is utilized in a number of applications, including in gas fuel storage, refrigeration and fluid separation. The compromises in designing adsorbent beds are complex, whereby materials with high porosity are preferable as they present a large surface area to the gas and can therefore adsorb a greater volume of gas to the surfaces. The adsorption phenomenon is exothermic and the the probability of a molecule being adsorbed decreases as temperature increases, with opposite occurring for desorption. This high dependency of adsorption with temperature and the poor thermal conductivity of porous materials hinders the overall process performance and require proper management. Apart from the usual distribution of fins along the domain for heat dissipation, this work introduces the concept of functionally graded adsorbent beds, with varying porosity and thermal conductivity across the domain. In this study, the transient Topology Optimization Method (TOM) is implemented to achieve optimal distributions of porosity regarding the storage of gas in porous materials by the adsorption phenomenon. The implementation is based on FEniCS and uses the Libadjoint library to calculate the full sensitivities. The formulation of the objective not only considers the maximum volume of gas which can be stored but also the time required to fill and empty the tank. Such a transient simulation requires the full description of the heat transfer, fluid dynamics and adsorption kinetics of both the absorption and desorption of the gas. In determining the distribution of material inside the domain, a material model based on Darcy law is employed, by using a permeability coefficient to alternate between the admissible material permeabilities. Resulting optimal porosity distributions for bidimensional design domains are presented with their gas storage metrics, as well as temperature and pressure distributions.