Thermochemical heat storage using silica gel offers high energy density, long storage, and minimal heat loss. While its performance is well–studied, the water binding within the gel and the storage mechanism require clarification. Using NMR, we analyzed water binding changes in silica gel before and after adsorption, defining the thermochemical reaction equation. Temperature and humidity's impact on adsorption was also examined. A theoretical heat storage density of 1029.63 kJ/kg was calculated, and kinetic analysis yielded an activation energy of 66.75 kJ/mol, suggesting a 3D diffusion model where water vapor diffusion in micropores is rate–limiting. Silica gel's heat storage density, ease of reaction, and cycling performance make it highly competitive.