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Insights into Cement Healing and Apparent Diffusivity Under Long-Term Carbonation: A Multi-Species Reactive Transport Model Approach

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A multi-species reactive transport model utilizing the non-iterative sequential method was created to assess the long-term effects of carbonation in cementitious materials. This study concentrated on the primary phases of hydrated G Class high sulfate-resistant grade, including Calcium Silicate Hydrate, Portlandite, Hydrotalcite, Monosulfoaluminate (AFm), C_3FH_6, and Ettringite (AFt). It was observed that higher pressures accelerate the CO_2 front propagation, particularly at elevated temperatures, though they do not significantly influence the extent of porosity changes. The effect of temperature is also analyzed, with a focus on CO_2 solubility, diffusivity, and mineral precipitation/dissolution. The results indicate that increasing the temperature from 25°C to 50°C has a minimal impact on CO_2 penetration depth, whereas at temperatures exceeding 50°C, the carbonation length increases significantly. Moreover, the study reveals that apparent diffusivity due to reactions and mineralization could decrease more than one order of magnitude, depending on the specific pressure and temperature conditions.