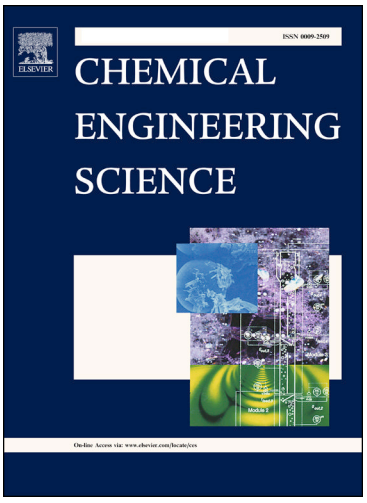

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Numerical and experimental study of La–Ni hydriding kinetics based on the varying-size model

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Abstract

Particle size often varies during gas–solid heterogeneous reactions. For example, metal hydrides (MH) can reversibly absorb and desorb H_2, accompanied by the expansion and shrinkage of the alloy particles, respectively. Although the traditional shrinking-core model (SCM) can be used to describe the H_2 absorption/desorption process, the calculation results from SCM show relatively large deviations from the experimental data without considering the factor of particle expansion/shrinkage. Therefore, we proposed a shrinking-core–varying-size model (SC-VSM, henceforth VSM) for MH particles that accurately determines the kinetics equation with particle deformation. Three types of control mechanism including H_2 dissociative chemisorption, H internal diffusion, and surface reaction were studied extensively, and the rate-controlling step for both VSM and SCM was determined to be the internal diffusion of H. Hydriding experiments on the systems of $LaNi_5$ and $LaNi_{4.5}Al_{0.5}$ were performed under quasi-isothermal and variable-pressure conditions. The simulation results indicated that the new VSM was highly consistent with the experimental data for both alloys, evidently providing higher precision than the traditional SCM. The simplified forms of the VSM diffusion equations for $LaNi_5$ and $LaNi_{4.5}Al_{0.5}$ were also developed to facilitate their practicability during the hydriding process:

$LaNi_5$: $1.426-1.419(1-X)^{\frac{2}{3}}-0.046(1-X)^{\frac{5}{3}}-0.95X+0.038(1-X)^2=\frac{t}{\tau'_{\mathrm{diff}}}$

$LaNi_{4.5}Al_{0.5}$: $1.362-1.35(1-X)^{\frac{2}{3}}-0.069(1-X)^{\frac{5}{3}}-0.90X+0.057(1-X)^2=\frac{t}{\tau'_{\mathrm{diff}}}$