Molecular Reaction Kinetic Mechanisms of Organic Pollutant Degradation in Coal Fire Combustion Processes

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Abstract

Coal fires in China are severe, and the tar produced by coal combustion is enriched with organic pollutants such as polycyclic aromatic hydrocarbons (PAHs), which not only severely harm the ecological environment but also exhibit "carcinogenic, teratogenic, and mutagenic" effects on humans. To address this, this study proposes an in-situ chemical activation degradation method for residual tar in coal fire zones. The degradation characteristics of organic pollutant components in residual tar under persulfate chemical activation were investigated, and the molecular reaction kinetics mechanism of chemical activation degradation for organic pollutants was elucidated. The results show that the optimal chemical activation time for degrading seven key PAHs in residual coal containing tar (heavy and light) is 24 h, with an optimal activation concentration of 35.70 mmol/L. In chemically activated coal containing heavy tar, the degradation rates of PAHs at different temperatures (300–500 ℃) followed the order: naphthalene > acenaphthene > fluorene > phenanthrene > anthracene > pyrene > fluoranthene. The degradation rate of naphthalene ranged between 46.88%–54.98%. For light tar-containing coal samples at 350 ℃, 450 ℃, and 500 ℃, acenaphthene exhibited the highest degradation rate, while anthracene had the lowest. In on-site fire zone contaminated soil, phenanthrene and anthracene accounted for the largest proportions, with degradation rates following the order: phenanthrene (57.28%) > naphthalene > acenaphthene > anthracene > pyrene > fluorene > fluoranthene. Molecular reaction kinetics revealed that SO_4^{-}• primarily attacks C-H bonds on PAHs, while •OH radicals target electron-rich carbon atoms on the central rings of PAHs. Through oxidative decarboxylation and ring-opening reactions, quinone or ketone intermediates are generated and eventually mineralized into CO_2 and H_2O. This research provides scientific insights for achieving synergistic management of coal fire extinguishing and organic pollution at the source, ensuring ecological safety in fire zones.

Keywords

Coal Fires, Organic Pollutants, In-Situ Chemical Activation, Polycyclic Aromatic Hydrocarbons (Pahs), Molecular Reaction Kinetics