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REACTION KINETICS, CATALYSIS AND……

碳酸钠促进选择性非催化还原脱硝的动力学模型与模拟

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摘要 The detailed kinetic model of selective non-catalytic reduction (SNCR) of nitric oxide, including sodium species reactions, was developed on the basis of recent studies on thermal DeNOx mechanism, NOxOUT mechanism and promotion mechanism of Na2CO3. The model was validated by comparison with several experimental findings, thus providing an effective tool for the primary and promoted SNCR process simulation. Experimental and simulated results show part-per-million level of sodium carbonate enhances NO removal efficiency and extend the effective SNCR temperature range in comparison with use of a nitrogen agent alone. The kinetic modeling, sensitivity and rate-of-production analysis suggest that the performance improvement can be explained as homogeneous sodium species reactions producing more reactive OH radicals. The net result of sodium species reactions is conversion of H2O and inactive HO2 radicals into reactive OH radicals, i.e. H2O+HO2＝3OH, which enhances the SNCR performance of nitrogen agents by mainly increasing the production rate of NH2 radicals. Moreover, N2O and CO are eliminated diversely via the reactions Na+N2O＝NaO+N2, NaO+CO＝Na+CO2 and NaO2+CO＝NaO+CO2, in the promoted SNCR process, especially in the NOxOUT process.

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Kinetic model and simulation of promoted selective non-catalytic reduction by sodium carbonate

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Abstract The detailed kinetic model of selective non-catalytic reduction (SNCR) of nitric oxide, including sodium species reactions, was developed on the basis of recent studies on thermal DeNOx mechanism, NOxOUT mechanism and promotion mechanism of Na2CO3. The model was validated by comparison with several experimental findings, thus providing an effective tool for the primary and promoted SNCR process simulation. Experimental and simulated results show part-per-million level of sodium carbonate enhances NO removal efficiency and extend the effective SNCR temperature range in comparison with use of a nitrogen agent alone. The kinetic modeling, sensitivity and rate-of-production analysis suggest that the performance improvement can be explained as homogeneous sodium species reactions producing more reactive OH radicals. The net result of sodium species reactions is conversion of H2O and inactive HO2 radicals into reactive OH radicals, i.e. H2O+HO2＝3OH, which enhances the SNCR performance of nitrogen agents by mainly increasing the production rate of NH2 radicals. Moreover, N2O and CO are eliminated diversely via the reactions Na+N2O＝NaO+N2, NaO+CO＝Na+CO2 and NaO2+CO＝NaO+CO2, in the promoted SNCR process, especially in the NOxOUT process.

Key words kinetic model; simulation; selective non-catalytic reduction; nitric oxide; sodium carbonate; mechanism

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