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Experimental and Modeling Study of The Mutual Oxidation of N-pentane and

Nitrogen Dioxide at Low and High Temperatures in a Jet Stirred Reactor

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Abstract: The mutual oxidation of n-pentane and NO₂ at 500-1000K has been studied at equivalence ratios of 0.5 and 1.33 by using an atmospheric-pressure jet stirred reactor (JSR). N-pentane, O₂, NO, NO₂, CO, CO₂, CH₂O, C₂H₄, and CH₃CHO are simultaneously quantified, in-situ by using an electron-impact molecular beam mass spectrometer (EI-MBMS), a micro-gas chromatograph (μ -GC), and a mid-IR dual-modulation faraday rotation spectrometer (DM-FRS). Both fuel lean and rich experiments show that, in 550-650K, NO₂ addition inhibits low temperature oxidation. With an increase of temperature to the negative temperature coefficient (NTC) region (650-750K), NO₂ addition weakens the NTC behavior. In 750-1000K, high temperature oxidation is accelerated with NO₂ addition and shifted to lower temperature. Two kinetic models, a newly developed RMG n-pentane/NO_x model and Zhao's n-pentane/NO_x model (Zhao et al. 2018, Submitted) were validated against experimental data. Both models were able to capture the

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