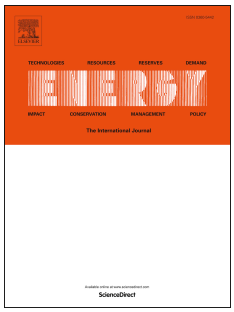
Accepted Manuscript



Experimental and modeling study of the mutual oxidation of *N*-pentane and nitrogen dioxide at low and high temperatures in a jet stirred reactor

Hao Zhao, Alon G. Dana, Zunhua Zhang, William H. Green, Yiguang Ju

PII: S0360-5442(18)31994-7

DOI: 10.1016/j.energy.2018.10.013

Reference: EGY 13910

To appear in: *Energy*

Received Date: 2 June 2018

Revised Date: 8 September 2018

Accepted Date: 2 October 2018

Please cite this article as: Zhao H, Dana AG, Zhang Z, Green WH, Ju Y, Experimental and modeling study of the mutual oxidation of *N*-pentane and nitrogen dioxide at low and high temperatures in a jet stirred reactor, *Energy* (2018), doi: https://doi.org/10.1016/j.energy.2018.10.013.

Experimental and Modeling Study of The Mutual Oxidation of N-pentane and Nitrogen Dioxide at Low and High Temperatures in a Jet Stirred Reactor

Hao Zhao[1], Alon G. Dana[2], Zunhua Zhang[1, 3], William H. Green[2], Yiguang Ju[1]*

[1]*Department of Mechanical and Aerospace Engineering,*

Princeton University, Princeton, NJ 08544-5263, USA

[2]*Department of Chemical Engineering,*

Massachusetts Institute of Technology, Cambridge, MA, 02139-4307, USA

[3]*School of Energy and Power Engineering,,*

Wuhan University of Technology, Wuhan 430063, China

[*]*Corresponding Author Email: haozhao@princeton.edu*

Abstract: The mutual oxidation of n-pentane and NO_2 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, O_2, NO, NO_2, CO, CO_2, CH_2O, C_2H_4, and CH_3CHO 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, NO_2 addition inhibits low temperature oxidation. With an increase of temperature to the negative temperature coefficient (NTC) region (650-750K), NO_2 addition weakens the NTC behavior. In 750-1000K, high temperature oxidation is accelerated with NO_2 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