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Experimental and modeling study of fuel interactions with an alkyl nitrate cetane enhancer, 2-ethyl-hexyl nitrate

S.S. Goldsborough^{a,b,*}, M.V. Johnson^a, C. Banyon^a, W.J. Pitz^c,
M.J. McNenly^c

^a Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439, USA

^b Department of Mechanical and Industrial Engineering, University of Illinois Chicago, Chicago, IL 60607, USA

^c Lawrence Livermore National Laboratory, Livermore, CA 94551, USA

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Abstract

This study investigates the autoignition behavior of two gasoline surrogates doped with an alkyl nitrate cetane enhancer, 2-ethyl-hexyl nitrate (2EHN) to better understand dopant interactions with the fuels, including influences of accelerating kinetic pathways and enhanced exothermicity. A primary reference fuel (PRF) blend of *n*-heptane/iso-octane, and a toluene reference fuel (TRF) blend of *n*-heptane/iso-octane/toluene are used where the aromatic fraction of the latter is set to 20% (liquid volume), while the content of *n*-heptane is adjusted so that the overall reactivity of the undoped fuels is similar, e.g., Anti-Knock Index (AKI) of ~91, Cetane Number (CN) ~25. Doping levels of 0.1, 1.0 and 3.0% (liquid volume basis) are used where tests are conducted within a rapid compression machine (RCM) at a compressed pressure of 21 bar, covering temperatures from 675 to 1025 K with stoichiometric fuel–oxygen ratios at O₂ = 11.4%.

At the experimental conditions, it is found that the doping effectiveness of 2EHN is fairly similar between the two fuels, though 2EHN is more effective in the aromatic blend at the lowest temperatures, while it is slightly more effective in the non-aromatic blend at intermediate temperatures. Kinetic modeling of the experiments indicates that although some of the reactivity trends can be captured using a detailed model, the extents of predicted Cetane Number enhancement by 2EHN are too large, while differences in fuel interactions for the two fuels result in excessive stimulation of the non-aromatic blend. Sensitivity analysis using the kinetic model indicates that the CH₂O and CH₃O₂ chemistry are very sensitive to the dopant at all conditions. The rate of 2EHN decomposition is only important at low temperatures where its decomposition rate is slow due to the high activation energy of the reaction. At higher temperatures, dopant-derived 3-heptyl radicals are predicted to play an important role stimulating ignition. Finally, nitrogen chemistry is important through the 'NO – NO₂ loop' where this can generate substantial amounts of OH. However, at the highest doping levels the formation of methyl and ethyl

* Corresponding author at: Energy Systems Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, USA. Fax: +1 630 252 3443.

E-mail address: scott.goldsborough@anl.gov (S.S. Goldsborough).

nitrite, and nitric acid significantly competes with this so that less OH is generated and this constrains the reactivity enhancement of 2EHN.

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1. Introduction

Alkyl nitrates are identified as effective fuel additives which can be used in very small quantities (e.g., 1–1000 ppm) to improve the ignition quality of ‘low grade’ fuels. Ignition quality is often designated using Cetane Number (CN) where high values, e.g., $CN > 60$, indicate very reactive fuels, such as those with significant amounts of linear paraffins, while low values, e.g., $CN < 30$, indicate less reactive fuels, such as ones with high iso-paraffinic or aromatic content. Low fuel reactivity can lead to problems in diesel combustion concerning power output, engine deposits, high emissions, rough operation, and cold starting. Fuel reactivity has also been identified as an important parameter influencing the performance and controllability of advanced combustion schemes, such as homogeneous charge compression ignition (HCCI) [1] and reactivity controlled compression ignition (RCCI) [2]. It has been suggested that fuel additives could be one way to dynamically control fuel reactivity during engine operation in order to cover a wide range of combustion modes.

Alkyl nitrates, and other cetane enhancers such as peroxides, e.g., di-tert-butyl peroxide (DTBP), are highly reactive compounds containing weak intramolecular bonds which lead to rapid decomposition at modest temperatures. This means that in practical combustors they break down early in the combustion process. Decomposition yields active chemical species; in the case of alkyl nitrates, alkyl radicals, aldehydes and nitrogen dioxide are formed. These products interact with the fuel and other gases, e.g., O_2 , to accelerate the ignition process. The early reactions often have some exothermicity and thus can provide a thermal stimulant to supplement the accelerating kinetic pathways. Alkyl nitrates are advantageous due to their low cost and chemical stability outside of the combustion chamber. Peroxides, for instance, can react with the fuel during storage resulting in increased rates of gum, varnish and sediment formation during engine operation.

Alkyl nitrates and peroxides have been investigated in fundamental experiments, as well as combustion engines, while a number of detailed theoretical and modeling studies have also been undertaken [3–17]. Single-shot spray chambers have been used [3], as have RCMs [4–6], shock tubes [7,8] and flow reactors [9]. Engine studies have utilized conventional and low temperature

combustion (LTC) direct injection schemes [10–12], as well as HCCI [13] and RCCI [14,15]. Chemical kinetic models have been developed to predict the decomposition behavior of 2EHN and DTBP [5,16,17], and the sensitizing effects they have on some fuels of interest, e.g., *n*-heptane [8].

Currently however, there is still a lack of fundamental understanding regarding a number of issues related to fuel additives, including:

1. How do additives interact with fuel components (e.g., paraffins, branched alkanes, aromatics, olefins, etc.) across a range of engine operating conditions?
2. What are the influences of exothermicity and accelerating kinetic pathways?
3. Can interactions and influences be reliably predicted, along with impacts to pollutant formation?
4. Are there optimal additives that can be used across a range of operating modes, including LTC?

The objective of this study is to provide insight into these questions. Experiments and modeling are conducted where tests are performed using an RCM. Two different gasoline surrogates are used in order to discern the influence of aromatic content on the effectiveness of 2EHN, while the overall level of reactivity is similar. Gasoline surrogates are employed here as opposed to diesel ones due to the relevance of gasoline to some LTC modes [12] as well as single-fuel RCCI [14,15] where cetane enhancers are of interest, while a relevant range of doping levels is explored. Chemical kinetic models are developed and simulations conducted of the RCM experiments. Sensitivity and rate-of-production (ROP) analyses are also performed to facilitate an understanding of the mechanistic interactions.

The rest of this paper is organized as follows. First, the experimental facilities and techniques are described, after which the kinetic model and simulation framework are discussed. The results are then presented, followed by a summary and conclusions of the current work.

2. Experimental

Argonne’s twin, opposed-piston RCM is used for this study. Its capabilities are detailed elsewhere [18], however a brief description is provided

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