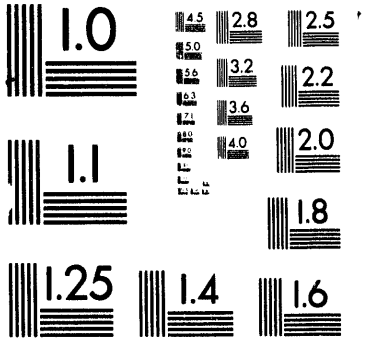
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10 January 1994

Mr. Tom Sebestyen
Office of Transportation Technologies
U.S. Department of Energy, Mail Stop 322
1000 Independence Avenue, S.W.
Washington, DC 20585

RE: "Fuel Property Effects on Engine Combustion Processes", DE-FG04-87AL44658, Annual Report: 1/1/93-12/31/93

Dear Tom:

The objectives of this program are to develop an understanding of the oxidation chemistry of combustion processes and to determine fuel property effects on these processes. The scope of the research program has been directed toward the study of the chemistry at low and intermediate temperatures with major emphasis placed on its relationship to autoignition, emissions and engine knock. Recently, in keeping with the general needs and research interests of the engine research community, the emphasis has been shifting more and more towards emissions, particularly hydrocarbon emissions. Efforts are being concentrated on autoignition chemistry; the role and significance of the preignition end gas reactions and heat release in autoignition and knock; pressure effects on hydrocarbon oxidation mechanisms; and fuel chemistry effects on hydrocarbon decomposition processes and emissions. The fuel chemistries investigated have included suggested additives and blending components for reformulated gasolines.

The approach being used to achieve these objectives is to conduct experiments primarily in an optically and physically accessed research engine on loan from Sandia National Laboratories. Bench scale facilities: a static reactor and an atmospheric pressure flow reactor, provide the flexibility to perform more fundamental chemical studies which complement the engine studies. A short description of the progress made during this reporting period follows.

Our engine studies have concentrated on 2 areas of interest to autoignition and emissions from engines. In the first, we investigated the effect of nitric oxide (NO) on the reactivity and autoignition behavior of 87 PRF. In the second study, we continued work on the effects of blending ethers on the reactivity and autoignition of a primary reference fuel blend, 87 PRF, with emphasis placed on the chemical interactions between ethers and the baseline fuel.

The effects of nitric oxide (NO) on the reactivity and autoignition behavior of 87 PRF were examined in our research engine under motored conditions at compression ratios of 5.2 and 8.2. The new compression ratio, 8.2, was obtained by modifying the "engine puck", allowing studies on autoignition behaviors of 87 PRF or higher octane fuels. Our experimental results show that, at low inlet manifold temperatures, low concentrations of nitric oxide promoted reactivity and high concentrations caused a significant decrease in reactivity. With an increase in manifold temperature, the promoting effect extended to higher NO concentrations. We observed that 400 ppm NO caused autoignition at a manifold temperature of 477 K whereas baseline fuel (0 ppm) did not autoignite even at

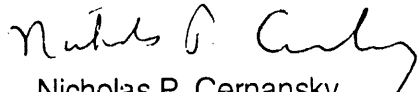
500 K. The most significant conclusions of our study are: i) nitric oxide does interact with the hydrocarbon oxidation at conditions typically experienced by the end gas in a fired engine; (ii) the effect is complex and, depending on the reaction environment, the same concentration of NO can produce dramatically different results. These results are particularly important given the fact that residual fractions and recycled exhaust gases in spark ignited engines typically result in about 200-600 ppm of NO in the unburned charge. Thus, future studies on the interactions of NO and hydrocarbon fuel chemistry are warranted. The results were presented at the SAE Fuels and Lubricants Meeting in Philadelphia, PA in October, 1993 as SAE Paper 932757.

The octane enhancing ethers, MTBE, ETBE, TAME, and DIPE, were blended into 87 PRF at a constant O atom fraction of 1.94% in the fuel mixtures and the mixtures were tested under motored conditions at our new compression ratio of 8.2. This new compression ratio allows studies on autoignition behaviors of 87 PRF with and without ethers. The results showed that, when using 87 PRF/ether mixtures, reactivity was significantly reduced as indicated by the higher inlet temperature required to initiate reactivity, significantly lower maximum CO concentration and the significantly higher inlet temperature required for autoignition. The magnitude of effects varied with the ether used. ETBE and MTBE were found to be the most effective ethers in inhibiting autoignition, followed by TAME, and finally DIPE. In-cylinder gas analyses were conducted using 87 PRF and its mixture with MTBE and DIPE, providing concentration profiles as a function of crank angle degree. The results of the in-cylinder gas analyses showed that ethers interact with 87 PRF principally by the creation of an active radical pool. This is indicated by the unchanged relative baseline fuel consumption rate and similar intermediate species concentration profiles. The ethers were effective in inhibiting autoignition because they consume the active radical pool generated by 87 PRF, substituting a relative stable pool of radical and intermediate species which reduces the overall reactivity. The reduced reactivity and unreacted ethers were responsible for the delay in autoignition. The results showed that the effects on reactivity and autoignition were not only determined by the ability of the ether to consume OH· radicals, but also by the ability of the radical formed from oxidation of the ethers to regenerate active radicals. These results will be presented at the SAE International Congress Meeting, Detroit, MI in February, 1994 as SAE paper 940478.

Following up studies of pentane in the engine, studies have commenced on the pre-ignition oxidation chemistry of olefins in the static reactor. Since 1-pentene is an important intermediate species during oxidation of pentane, it has been selected for initial study. Over the first half of 1993, static reactor system verification and testing were conducted. A few changes were made in the experimental set-up, and the system behavior was confirmed by experiments with propane. Subsequently, we conducted an overall reactivity mapping of 1-pentene and measured pressure-temperature profiles at various initial pressures and temperatures and at different equivalence ratios. These data are useful in selecting conditions for detailed speciation studies. Presently, we are measuring the species profiles during oxidation of 1-pentene at 0.8 equivalence ratio, and at various initial temperatures and pressures. Once this is done, species data will be obtained at other equivalence ratios.

Please feel free to contact me at (215)-895-2284 if you have any comments or questions.

Sincerely



Nicholas P. Cernansky
Hess Chair Professor
Principal Investigator

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END