REQUIREMENTS FOR THE FUTURE AVIATION JET FUEL TO BE DEVELOPED BY MOLECULAR ENGINEERING OF LIQUID HYDROCARBON FRACTIONS

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Abstract

Requirements for the molecular basis of the future aviation jet fuel will be discussed and the work going on in Finland for this goal will be reviewed. The most important environmental aspects are efficient combustion performance for suppressing formation of toxic compounds like nitrogen oxides and certain polycyclic aromatic hydrocarbons. The most harmful uncompleted combustion products are carbon containing nanoparticles that contain adsorbed nitrogen oxides and carcinogenic aromatic compounds. Therefore fuel combustion cleanliness is one of the most important goal in our investigations not only because of our health but also because of the cleanliness of critical fuel system components and the engine. These objectives together with the need of adding molecular specifications for the future fuel are discussed.

Introduction

The most important requirement for the future aviation jet fuel is to conserve the existing operational and handling safety of the present kerosene based fuels. Hydrogen and other gaseous or liquid low-boiling fuels require much more efforts to prevent fuel leakages and other safety arrangements in any accidental functional problems of the fuel system. Therefore, it is very likely that the jet fuel beyond the year 2000 will be a modified kerosene manufactured from crude oil, natural gas, coal or any carbon and hydrogen containing stock or waste material. This solution would be the most efficient for every day air traffic with jet engine air craft and also for the majority of the military air craft.

The necessary practical properties specified or otherwise important for commercial and military fuels like necessary chemical, physical and biological stability, clean combustion for the engine and environment, lubricity and corrosion prevention for the fuel system, conductivity to prevent electrical discharges, proper viscosity in different temperatures, proper temperature conductivity and cooling capacity for engine lubricant and other fuel cooled aircraft components and finally anti-icing property to prevent formation of ice crystals at low temperatures are presently obtained by formulating the kerosene fraction with several approved additives. In the future the above properties of the fuel will be most likely introduced to the kerosene in the fuel processing and therefore no or much less additives would be needed. This approach will simplify the fuel handling and logistics because specific fuel properties can be tailored in the refineries by molecular engineering of the kerosenes. There are several advantages of this approach because water separation will become unnecessary due to the controlled water solving properties of the fuel and fuel compatibility with different types of engines, fuel system seals and any acceptable operating conditions.

The aim of this paper is to describe requirements for the future kerosene fuels on the basis the research work carried out several years in Finland and recently in a close cooperation with Finnish Air Force. The general approach has been to investigate and develop analytical methods for complete characterization of each of the hundreds of energy producing compounds of kerosenes as well as molecular structure and reaction mechanisms of natural and additive trace compounds that make kerosenes acceptable as the specified Jet A-1 or JP-8 fuels.

It is natural that new molecular specifications are needed in the future to achieve the perfect control of fuel performance in all conditions. Therefore, another goal of our research work is to develop chromatographic conditions for adequate separation of all jet fuel compounds that have significance on fuel behavior and specifications and, on the other hand, the development of retention index library for fuel compounds to make possible in the future an automated monitoring of molecular specifications of jet fuel compounds for principal energy producing molecules and for principal trace property molecules like stability, combustion, lubricity, anti-icing, conductivity etc. The complexity of kerosene fuels requires the use of hyphenated techniques like the two-stage retention index monitoring HRGC (RIM/RIM) method what we have earlier used for monitoring benzene from gasoline. In development of RIM/RIM library mass spectrometric detection is necessary together with the high field NMR analysis of fuel fractions. The routine system would however be most likely based on HRGC/RIM/RIM with flame ionization detection (FID).[1-3]

Experimental

Several Jet-A1 and JP-8 samples based on different kerosenes were analyzed using high resolution gas chromatography (HRGC), HRGC-mass spectrometry (MS) and high field nuclear magnetic resonance (NMR) spectrometry methods. Instruments used were Micromat HRGC 412 with two 15 m capillary columns (a cyanopropyl NB-1701 and a phenyl methyl silicone NB-30) and two flame ionization detectors (HNU Nordion) and Hewlett-Packard HP 5890 GC with HP 5970A Series Mass Selective Detector (MSD). Some samples were analyzed just as obtained from the refinery (Neste Oy), some of samples were of different age (Finnish Air Force) and one sample (Sabena Air Lines Depot) was allowed to stand up to two and half years before analysis. Some samples were also oxidized by bubbling air or oxygen through the fuel to follow the formation of oxidation products.[4] NMR instrument used was Varian Unity 600 operating at 600 MHz for protons and at 150 MHz for carbon-13 measurements.

Results and Discussion

Jet fuel specifications were studied with the objective of elucidating chemical reaction mechanisms and physical interactions that determine the behavior of fuel as whole material and how individual major and trace compounds produce this bulk behavior for the fuel. Because some natural trace molecules and additives are extremely important in fuel performance careful library and patent search was carried out about these molecules and their functioning in combustion and fuel system was elucidated together with our own experimental work.

The most important result of this work is the critical evaluation of environmental aspects of jet fuel combustion. A conclusion was made on the basis of medical reasons. It is known that combustion exhaust of jet engine produces more or less small particles and gaseous contaminants from which nitrogen oxides and some polycyclic aromatic hydrocarbons are the most harmful. Amount and quality of these harmful exhausts depend on type and functioning of engine and amount of power taken from the engine at a moment of time and also on the chemical composition of the fuel.

While carbon dioxide has also been mentioned as a harmful exhaust it is not toxic and we consider it therefore as of the secondary importance. A sooting flame of jet engine produces visible particles of micron size or more but a non-sooting flame may also produce small nanometer scale particle that are not visible but may be even more harmful because of larger surface area which may be occupied by carcinogenic molecules. Therefore in the future the combustion should be perfect with any type of engines, with single or two-stage combustion zones, producing only carbon dioxide and water as the combustion products. This means that both the future engines and future fuels should be optimized and jointly developed. The fuel should be free of harmful trace elements and contain structural groups which enhance clean and efficient combustion without producing harmful deposits or other products.

Another important fuel property is its lubrication capability. Fuel is the only lubricant of fuel pumping system and the whole line of fuel system components up to the injector nozzle. It should therefore have an adequate corrosion inhibition and boundary lubrication behavior which works mainly through surface active alkyl phenols and carboxylic acids derivatives which are natural or additive trace molecules. We have studied commercial diesel fuels for boundary lubricants and use this data also for designing adequate lubricity for the future green jet fuel.[5]

Autooxidative, surface catalytic, pyrolytic and mechanochemical stability of fuel at high temperatures and the other necessary properties should on the basis of the above discussion be obtained by molecular tailoring of the fuel production process. With the present knowledge about catalysis these process modifications are realistic and cost effective so that production costs of the future green fuel will not be significantly higher compared to the present fuels.

To guide this work and also to make possible future fuel quality monitoring molecular specifications are needed and for this purpose we develop an automated sample preparation HRGC-RIM/RIM -system that can be used by oil companies, air line companies and military operators. Molecular procedure based on high field NMR and HRGC are being developed to automatically determine combustion index, lubricity index, and fuel stability index from the analytical data. These figures are naturally calibrated with bulk property tests which data are used for refinement of fuel specification index calculations. This research and development work is going on in Finland and the first results will be a prototype green fuel according to the above guidelines and a prototype molecular level fuel analyzer.

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