Project 031(B) Methods for the Fast Quantification of Oxygenated Compounds in Alternative Jet Fuels

Washington State University

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University Participants

Washington State University
- P.I.(s): Manuel Garcia-Perez
- FAA Award Number: 13CAJFEWaSU-008
- Period of Performance: July 1st, 2016, to June 30th, 2017
- Task(s):
  1. Literature review
  2. Improving the method for quantification of independent oxygenated compounds in AJFs
  3. Development of methods for the fast quantification of oxygenated compounds in jet fuels

Project Funding Level
Washington State University: Amount of funding from the FAA ($ 50,963), Matching funds ($ 51,130), Source: State Funds to support one graduate student (from Dr. Cavalieri’s program) and Dr. Garcia-Perez’s salary.

Investigation Team

Yinglei Han (PhD student): Improving the methods for quantification of independent oxygenated compounds in AJFs

Mainali Kalidas (MSc student): Literature review and development of methods for the fast quantification of oxygenated compounds in jet fuels

Manuel Garcia-Perez (Associate Professor): Principal Investigator, project management and reporting

Project Overview

The studies conducted last year show that the chemical compositions of the alternative jet fuels studied (SK and SAK from Virent, Kior, Gevo, Amyris, and ARA; HEFA from UOP, FT from Sasol and Syntroleum) range from fuels comprised of single molecules to fuels with thousands of molecules with a wide range of molecular weights and functionalities. These fuels have contents of trace oxygenated molecules similar to commercial jet fuels, but the types of oxygen groups are fuel dependent. This year we want to continue the work we started last year but focusing on improving the method for the quantification of oxygenated compounds and developing fast detection methods for oxygenated functional groups that can be used during AJF production or at distribution and blending points to control fuel quality.
Tasks

Task 1. Literature review
Washington State University

Objective(s)
To conduct a literature review on the methods for the quantification of oxygenated compounds in alternative jet fuels.

Research Approach
We conducted a literature review on methods for the quantification of oxygenated compounds in alternative jet fuels. The main goal of this task is to review the methods available for the quantification of total functional groups (acids, carbonyl, phenols) and the methods for the quantification of independent compounds in alternative jet fuels. We also reviewed methods that can be potentially used for the quantification of targeted oxygenated compounds in organic matrices.

Milestone(s)
The literature review has been completed and it is now under internal review.

Major Accomplishments
The first draft of the literature review has been completed.

Publications
None

Outreach Efforts
None

Awards
None

Student Involvement
A MSc student (Mainali Kalidas) conducted this literature review.

Plans for Next Period
Prepare a presentation with the main outcomes of this literature review for our first 2017 ASCENT workshop.

Task 2 Improving the method for quantification of independent oxygenated compounds in AJFs
Washington State University

Objective(s)
Validation of Balster’s method (Balster et al 2006) for the quantification of oxygenated compounds in AJFs.

Research Approach
In the first year of this project we quantified the content of individual oxygenated compounds by the method described by Balster et al. (2006). The polar molecules were concentrated through Solid phase Extraction (SPE) using a 6 mL Agilent SamplIQ silica SPE cartridge. 10 mL sample of jet fuel was analyzed per run. A volume of 12 mL hexane was used to rinse the cartridge and after that 11 mL of methanol eluted to polar species. The samples collected from SPE were then analyzed by GC/MS. Both internal and external standards were used for the analysis. This method was validated with new standards.
this year. The main question we want to answer is if all the oxygenated compounds adsorbed on the SPE cartridge were in fact removed with the methanol and to confirm that the quantitative results are reliable.

**Milestone(s)**
Studies were conducted with several bio-oil methanol ratios, with jet fuels doped with several phenols. In all cases the recovery obtained was close to 100 %, confirming that all the oxygenated compounds retained in the Silica SPE cartridge can be recovered with methanol.

**Major Accomplishments**
We confirmed that the method proposed by Balster et al (2006) is a reliable quantitative approach for the quantification of polar oxygenated compounds in jet fuel.

**Publications**
None

**Outreach Efforts**
None

**Awards**
None

**Student Involvement**
Two graduate students (Yinglei Han and Kalidas Mainali) worked on this task.

**Plans for Next Period**
To prepare the presentation for the first 2017 ASCENT workshop.

**Task 3 Development of Methods for the Fast Quantification of Oxygenated Compounds in Jet Fuels**
Washington State University

**Objective(s)**
Develop a method for the fast quantification of oxygenated functional groups in alternative jet fuels

**Research Approach**
The third task consists on studies to develop methods for the fast quantification of oxygenated functional groups in alternative jet fuels (E411 2012, Christiensen et al. 2011). The goal is to develop fast detection kits that can be used on field conditions. We will focus on the development of kits for the analysis of total carbonyl, total acids, and total phenols by spectroscopic and electrochemical techniques that can be easily miniaturized (Kauffman 1998, Qian et al 2008, Galuszka et al 2013, Novakova and Vickova 2009, Saito et al 2002, Tobiszewski et al 2009).

**Milestone(s)**
In the last six months we have been developing a strategy to quantify oxygenated compounds that used the extraction of the oxygenated compounds in methanol in a similar way that is done by the method proposed by Balster et al (2006) but after absorbing the polar compound silica cartridge is washed with hexane and to remove the jet fuel non polar molecules left on the cartridge. A washing step with methanol follows to obtain a solution of methanol with jet fuel polar compound in the ppm range. The resulting methanol solution was analyzed by UV-Fluorescence.
Major Accomplishments

A new method based on the analysis of methanol solutions containing jet fuel polar compounds by UV fluorescence has been developed. The appropriate jet fuel/silica/hexane/methanol ratio was determined to ensure a content of polar compounds in the resulting methanol solution below 5 ppm. This low concentration is needed to ensure a linear response of the UV-Fluorescence spectra to the changes in the concentration of polar compounds. Jet fuel doped with phenolic compounds were tested and the response obtained was in all cases linear. We are currently studying the response of other compounds found in the GC/MS chromatograms of the alternative jet fuel polar compounds.

Publications

None

Outreach Efforts

We are now working on the presentation for the first 2017 ASCENT workshop.

Awards

None

Student Involvement

This task was conducted by our MSc student Mainali Kalidas.

Plans for Next Period

We will conduct studies with other polar compounds found in alternative jet fuels.

References:


Kauffman RE: Rapid, Potable Voltammetric Techniques for Performing Antioxidant, Total Acid Number (TAN) and Total Base Number (TBN) Measurements. *Lubrication Engineering* 54.1 (1998), 39


