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## 2 Short communication

## Water solubility characteristics of current aviation jet fuels

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## ABSTRACT

Water solubility-temperature curves were created experimentally for five kerosine fuels and one widecut fuel. The Karl Fischer Coulometer method was used to determine the saturated water content of each fuel over a range of temperatures between -5 °C and 25 °C. The affinity for water of each fuel with respect to the other fuels was measured and ranked. The experimental solubility curves are comparable to the water solubility curves of the Jet A-1 and JP-4 fuels reported in the *CRC Handbook of Aviation Fuel Properties.* There are subtle differences between the experimental solubility curves and the CRC curves. This may be attributed to batch-to-batch variation or recent changes in fuel chemistry owing to the need to exploit less favourable crude oil reserves. A generic equation has been proposed to estimate the water solubility when aromatics content and flash point are known.

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1. Introduction

Jet fuel does not have an exact chemical composition; it is pro-40 41 duced to meet a set of properties defined by various specifications [1–5]. Its chemical composition will depend on the chemical spe-42 cies present in the parent crude oil that distil during the physical 43 separation in the kerosine boiling range and on further chemical 44 treatments that may be required to meet the jet fuel specifications. 45 46 The lack of precise property data is due to the variation of jet fuels, 47 based on the composition of the original crude oil and the refinery 48 methods used.

The three major constituent groups of jet fuel are paraffins (sat-49 urated alkanes), naphthenes (saturated cyclic alkanes) and aromat-50 ics [6-8]. The proportion of each chemical species varies from 51 52 batch to batch, but paraffins and naphthenes together account for a minimum of 70%v/v [8]. Aromatics are limited to a maximum 53 of 25%v/v [1] by specifications and to an industry accepted mini-54 55 mum of 8% v/v [6] for jet fuels containing synthetic components 56 conforming to the ASTM D7566-13 [9] specification. Olefins 57 (unsaturated hydrocarbons or alkanes) and trace impurities account for less than 5%v/v [8] and are minor constituents of jet 58 fuel. Baena-Zambrana et al. [10] provide an overview of the struc-59 ture of these classes of hydrocarbons. Further details may be found 60 in Hemighaus et al. [7]. 61

Aromatics are unsaturated hydrocarbons and have characteristic benzene rings with delocalized  $\pi$  electron clouds. They are

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http://dx.doi.org/10.1016/j.fuel.2014.04.091 0016-2361/© 2014 Published by Elsevier Ltd. mainly alkyl-benzenes and alkyl-naphthalenes [8]. It has been recognised that extended  $\pi$  electron systems such as those encountered in aromatics, form hydrogen bonds with water [11–13]. The formation of attractive electrostatic interactions between water and extended  $\pi$  electron systems account for the enhanced solubility of water in aromatics relative to both paraffins and naphthenes.

Water contamination of jet fuel can result in fuel system icing [14], microbial contamination, corrosion and tank gauging problems. Mathematical models have been developed for studying and predicting the dispersal of water in aircraft fuel systems [15,16], and are used in design to optimise fuel-water management and ensure that water build up is minimised throughout the system. These models compute the water contamination, due to the principal mechanisms of dissolution, suspension, condensation and transportation. Among other parameters, it is important to have accurate data on the water solubility behaviour in jet fuel to ensure confidence in the model results.

Some data on the water solubility behaviour in jet fuel are available in the open literature but this mostly dates back to the 1950s. Even data given in the *CRC Handbook of Aviation Fuel Properties* [6, Figs. 2–32], were found to pre-date 1984; the actual source of these data could not be verified but look similar to data presented by [17]. To take account of recent changes in fuel chemistry owing to the need to exploit less favourable crude oil reserves [18] and the introduction of non-petroleum-derived fuels, such as Fischer–Tropsch (FT), hydrotreated esters and fatty acids (HEFA) together with other alternatives [19–24], data on the water uptake and solubility in jet fuels needed to be updated. This study was used

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Abbre	viations	
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AVTAG	aviation wi de-cut turbine fuel	HEFA	hydrotreated esters and fatty acids
AVTUR	aviation turbine fuel	IBP	initial boiling point
COA Certificate of Analysis		KF	Karl Fischer
CRC Coordinating Research Council, Inc.		MSEP	Microseparometer
CTL	coal to liquid	NATO	North Atlantic Treaty Organisation
Di-EGMME Di-Ethylene Glycol Mono-Methyl Ether		PPMCC	Pearson product-moment correlation coefficient
FBP final boiling point		RH	relative humidity
FSII	fuel system icing inhibitor	SDA	static dissipater additive
FT	Fischer–Tropsch	UV	ultraviolet
GTL	gas to liquid		

to assess the water solubility of current aviation jet fuels to fill thatknowledge gap.

## 95 2. Test fuels

96 The study evaluated the water solubility characteristics of five 97 jet fuels made to different national standards, which either com-98 plied with or were very similar to the let A-1 fuel specification. The fuels were freshly sourced since fuel compositions may change 99 subtly with storage due to the formation of polar oxidation com-100 101 pounds such as organic acids. One of the fuels was fully synthetic, 102 i.e., not derived from conventional crude oil stocks. The work programme also included limited tests on a wide-cut fuel conforming 103 to the IP-4 specification; this contains a proportion of lighter 104 hydrocarbon molecules (naphtha or gasoline fraction). The lighter 105 106 fraction improves the fuel relight ability at altitude and reduces 107 its freezing point but also contributes significantly to the fire risk 108 due to a low flash point and higher vapour pressure. It is now only 109 used in consistently cold climates and availability is limited.

The fuels used in this study are summarised in Table 1. Fuels A
to E may be collectively referred to as kerosine fuels; Fuel F may be
referred to as a wide-cut fuel.

113 A Certificate of Analysis (COA) was supplied with each fuel as evidence that the fuel conformed to the relevant specification. 114 115 Chemical composition data and physical test data were given in 116 the COA. Some key characteristics of the test fuels are listed in 117 Table 2. The fuels were supplied to the normal commercial specifi-118 cation and included static dissipater additive (SDA), where shown. Fuel F was actually supplied to the NATO F-40 (AVTAG/FSII) spec-119 ification which includes requirements for lubricity improver, SDA 120 and fuel system icing inhibitor, FSII. 121

#### 122 3. Experimental

Fuels were filtered using nitrogen gas pressure through a
 Sartorius filter assembly fitted with Millipore HAWP04700
 (0.45 μm) mixed cellulose filter; fuels were filtered in batches of

Table 1

Test fuels.					
ID	Fuel & Specification	Provenance			
Α	Sasol Fischer–Tropsch fully synthetic Jet A-1	Sasol, South Africa			
В	Chinese No. 3 jet fuel	PetroChina International (Hong Kong) Ltd., Hong Kong			
С	Coryton high aromatics Jet A-1	Coryton Advanced Fuels Ltd., UK			
D	Air BP filton airfield Jet A-1	Air BP UK Ltd., Filton, UK			
Е	Russian TS-1 aviation kerosine	Blended by Coryton; tested/approved in Russia			
F	JP-4 wide-cut fuel	Coryton Advanced Fuels Ltd., UK			

approximately 1.2 l. Filtered fuels were stored in individual desic-126 cators and dried over silica gel for at least 24 h. This procedure 127 ensured that all the fuels had low concentrations of water initially 128 and that re-humidification below ambient temperatures could be 129 carried out without precipitating water. The desiccators were 130 stored inside a fume cupboard to minimise exposure to ambient 131 light. Fuel B was noted to be particularly susceptible to UV degra-132 dation, turning a noticeable yellow after a few days. The cause is 133 unknown but many studies have shown that photo-induced degra-134 dation may be a result of photo-oxidation and microbial degrada-135 tion [25-29]. 136

The fuels were re-humidified in a closed vessel (a desiccator containing a small amount of distiled water throughout the process) at the appropriate test temperature; the aim was to achieve a 100% relative humidity (RH) environment without introducing free water. A Mercia Scientific Humidicab was used for tests at or above 5 °C, as shown in Fig. 1, and a Fisons FE 300H cabinet for temperatures below 5 °C. To avoid over-saturating the fuels, each dried fuel sample was cooled to below the nominal conditioning temperature, transferred to the desiccator containing a small amount of distiled water and allowed to warm to the test temperature. Approximately 300 ml of fuel was treated in this way for each test. Fuel samples were gently stirred with a magnetic stirrer and the sample left to reach water saturated equilibrium at the relevant set temperature for at least 16 h. Previous work had shown this to be sufficient time for the system to reach equilibrium [30]. The desiccators were fitted with septum caps to allow sampling of the fuel without disturbing the equilibrium. A thermocouple was located in the fuel so that an accurate reading of the fuel temperature could be taken when sampled.

Karl Fischer (KF) coulometric titration with a Metrohm KF831 Coulometer was used to make the measurement of water in fuel. There are a number of test standards covering the use of KF Coulometers, but the most relevant in the context of fuel testing are ASTM E203 [31] and ASTM D6304 [32]. An SGE gas-tight 2.5 ml glass syringe with a long stainless steel luer needle was used for all injections. The Metrohm Karl Fischer Coulometer with an SGE glass syringe is depicted in Fig. 2. A multiple injection sequence with the needle tip below the surface of the anolyte was used for making the measurements (see A). The multiple injection procedure had been shown to give a smaller spread of results than the standard single injection technique. Type AG-H anolyte solution manufactured by Sigma Aldrich under the Hydranal Coulomat brand was used in the coulometer cell. It gave the most consistent results, with the least tendency to form a biphasic solution of fuel and anolyte.

## 4. Results and discussion

To generate the water solubility curves, the saturated water 173 content of each fuel was measured at nominal temperatures of 174

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