



Determination of hydrogen content in fuels by the method low resolution nuclear magnetic resonance spectroscopy (ASTM D7171-05 standard)

1. Introduction

The hydrogen content (HC) is the most important quality parameter of aviation fuels that is correlating with many of technical characteristics of this product. Essential properties of fuel combustion are primarily related to the total hydrogen content and non-optimal hydrogen content leads to the formation of carbon deposits, an increased amount of exhaust gases and smoke, as well as an increase in heat generation, which can lead to destruction of combustion chambers.

The method of pulsed nuclear magnetic resonance (NMR) is the simplest and most accurate one to measure the HC value.

advantages of the NMR method are:

- **Very simple and fast sample preparation;**
- **High accuracy and repeatability;**
- **No need in frequent calibrations;**
- **Non-destructive analysis allows repeated measurements;**
- **Short measurement time.**

2. Basics of the Method

After a sample is excited by a powerful 90° radio frequency pulse, the FID (free induction decay) signal is recorded. FID - is an electrical signal registered by the receiving part of the device. It accompanies the process of relaxation of magnetic moments of hydrogen nuclei protons — the return of spin system to an equilibrium state after radio-frequency excitation. The amplitude of a FID signal is directly proportional to the number of protons in sample. Thus, the NMR analyzer can be linearly calibrated for reference substances with known hydrogen content (Table 1).

Table 1. Reference substances with known hydrogen content

Substance	Hydrogen content, %
3- Cyclohexane propionic acid	10,324
Cyclohexylacetate	9,924
Malonic acid diethyl ester	7,552
Dodecane	15,386
Ethyl capronate	12,077
Ethylheptanoate	11,466
2- Nonanol	12,756
Octylacetate	11,703
Pentadecane	15,185
2- phenylethyl acetate	7,367

ASTM D7171-05 standard was developed to replace the ASTM D3701-01 and D4808-01 standards, since pulse NMR is faster and more accurate than the continuous sweep method.

3. Recommended Equipment

Time Domain NMR Analyzer «Spin Track» (pic. 1), produced by Resonance Systems, in the following configuration:



Pic 1. «Spin Track» NMR Analyzer

- Analyzer with thermally stabilized magnetic system (induction 0.4 - 0.5 T, gap for using the sensor with a test tube with a diameter of 18 mm *);
- Controlling PC with the pre-installed Microsoft OS © Windows 7, 8 or 10 ** and Relax 8 software;
- Thermostat "ST-80";
- Test tubes with outer diameter of 18 mm;
- Teflon caps for test tubes;
- Standards for validation.

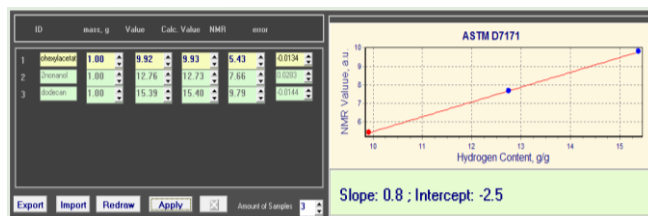
* Standard requirement

** Determined by the PC manufacturer

The Spin Track NMR analyzer is extremely easy to use and maintain, as measurement and validation procedures are maximally automated. Such accessories as Electronic Analytical Scales, automatic liquid dispenser, reference substances can be included in the delivery set.

4. Measurement and Calibration

The analyzer is calibrated with 2 or more substances from Table 1 by comparing the known mass fraction of hydrogen to the amplitude of the NMR signal. The calibration curve constructed using cyclohexyl acetate, 2-nonanol and dodecane is shown in pic. 2

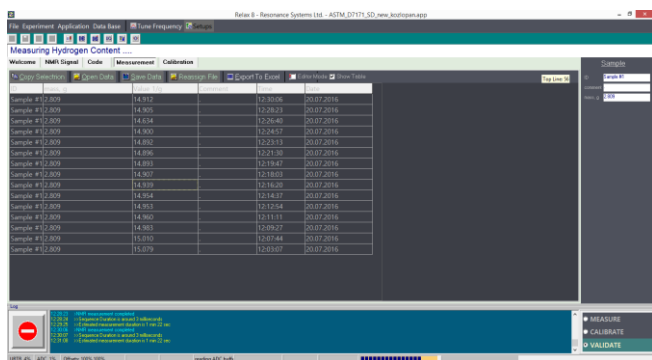


Pic 2. «Spin Track» NMR Analyzer Calibration Curve

Sample preparation is as simple as to put a fixed volume (following the manufacturer's instructions) of the test substance in a test tube using dispenser and determining its mass. The test tube with the sample is kept in a thermostat that maintains the temperature equal to the temperature of the magnetic system for at least 20 minutes. Next, the tube is placed into the Spin Track sensor and in less than 1 minute the HC value is displayed



automatically with the standard accuracy of 0.01% adding the record in electronic journal of measurements. (pic. 3). The software allows operation in the following modes: calibration, measurement and validation (estimation of reproducibility).



Pic. 3. The working window of the program Relax 8.0 with the loaded methodology (electronic measurement log).

The NMR analyzer is supplied with a pre-installed measurement program Relax8 and with tuned operational parameters. The device installation consists only in bringing the sample and magnet thermostats to the operating mode (about 4 hours). For more detailed information about the method, characteristics of the equipment and the capabilities of the software, please contact Resonance Systems directly at www.nmr-design.com.

5. Contacts

German Headquarter

Seestrasse 28, D-73230, Kirchheim/Teck, Resonance Systems GmbH
Fon: +49 (0) 7021-9822668, Fax: +49 (0) 7021-9822667,
Mobil: +49 (0) 172-4374693
E-mail: info@nmr-design.com

Czech Headquarter

Veleslavinska 39/48, Praha 6, 16200, Prague, Czech Republic, Resonance Systems s.r.o.
Tel.: +420 777 223 119
E-mail: info@nmr-design.com

Russian Headquarter

424000, Russian Federation, Mary El, Yoshkar-Ola, Volga State Technological University, Lenin sq., 3, Physics department, Resonance Systems Ltd.
Phones: +7 8362 532799, +7 8362 436020
E-mail: info@nmr-design.com