Automated preparation of surrogate mixtures for the determination of octane and cetane numbers

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Metrohm
Ion analysis

Titration

Summary

Commercially available fuels are complex mixtures of hundreds of different hydrocarbons. For the calibration of the test engines or advanced experimental and computational research they are modeled by means of multicomponent surrogate mixtures that adequately represent the desired physical and chemical characteristics.

By definition, every octane and cetane number corresponds to a specific mixing ratio of primary reference fuels (PRFs). Based on this information, the ***tiamo***™ controlled automatic dosing device prepares the surrogate mixtures. The setup drastically minimizes time-consuming and error-prone manual preparation steps and the contact with hazardous solvents. Additionally, precise and accurate results are displayed on customizable reports that fully comply with all current GLP and GMP requirements.

Introduction

The octane rating of gasoline is a parameter that indicates how much a fuel can be compressed before it spontaneously ignites. This spontaneous ignition is also known as engine knocking and adversely affects engine performance. The higher the octane rating of gasoline, the higher the resistance to knocking. By definition the octane rating of isooctane, a highly branched alkane that burns smoothly, is set to 100. The rating of n-heptane, an unbranched alkane that strongly tends to premature ignition, is set to zero. An octane rating of 85 means that the fuel has the same knocking properties as a mixture of 85% isooctane and 15% n-heptane.

There are different octane ratings such as the Research Octane Number (RON) or the Motor Octane Number (MON). Both of them are determined by using the fuel on a test engine (such as the CFR ASTM Test Engine) and comparing the obtained results with those for mixtures of isooctane and n-heptane. The different ratings result in different working conditions of the test engine. As the preparation of the solvent mixtures significantly affects the accuracy of the determination of the octane rating, strictly accurate solvent mixtures are of paramount importance.

This communication describes how PC-controlled automatic dosing devices allow a straightforward, reproducible and accurate preparation of solvent mixtures. Additionally, the manual handling with hazardous solvents is minimized, which translates into increased operator safety.

Instrumentation

- 846 Dosing Interface
- Dosino 800
- Dosing Unit
- 840 Touch Control

Surrogate mixtures

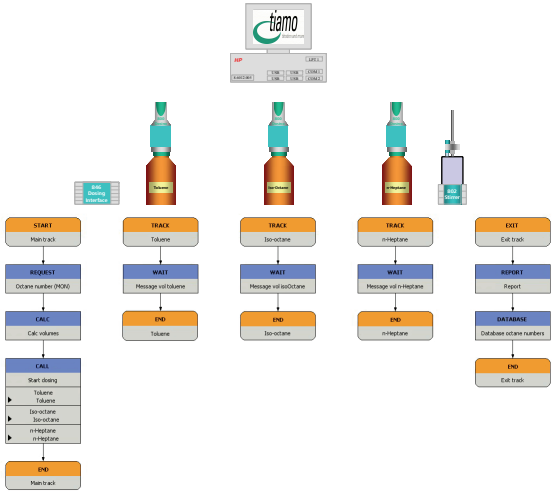
The wide range of hydrocarbon species in commercial gasoline complicates the understanding of fundamental physical and chemical processes in the test engine. A substantial number of surrogate mixtures, mainly consisting of the primary reference fuels (PRFs) n-heptane, iso-octane and toluene have been especially developed to mimic concrete fuel properties.

The calibration of internal combustion engines used for measuring the Motor Octane Numbers (MONs) of gasoline, for example, requires the accurate preparation of a high number of surrogate mixtures with known MON.

Motor Octane Number (MON)	Toluene [mL]	iso-Octane [mL]	n-Heptane [mL]
57.8	50	0	50
60.1	52	0	48
62.2	54	0	46
64.4	56	0	44
66.5	58	0	42
⋮	⋮	⋮	⋮
84.1	74	4	22
⋮	⋮	⋮	⋮
95.1	74	18	8
96.8	74	20	6
98.2	74	22	4
99.5	74	24	2
100.8	74	26	0

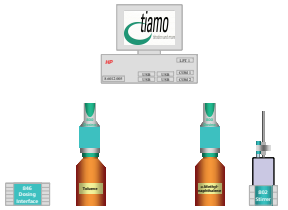
Preparation of fuel surrogate mixtures

An automated dosing system that is fully controlled by ***tiamo***™ replaces the tedious, time-consuming and error-prone manual preparation of surrogate mixtures.



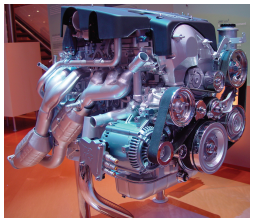
Preparation of diesel surrogate mixtures

Whereas for gasoline the desirable property is the ability to resist ignition when injected into the engine, the desired property of diesel fuel is to autoignite. The relevant parameter is the cetane number. A compound that has a high octane number tends to have a low cetane number. Binary surrogate mixtures, consisting of the PRFs cetane and α-methylnaphthalene are needed to adequately describe the chemical complexity of conventional diesel fuels.



Advantages

- Upgradable custom-designed setup – surrogate mixtures of numerous primary reference fuels can be prepared
- Preparation of variable sample volumes between 0.1…1 L
- Fully automated dosing minimizes manual handling with hazardous solvents
- Accurate and precise dosing provide highly reproducible surrogate mixtures
- Detailed and customizable reports are in accordance with GLP and GMP
- Parallel dosing of the primary reference fuels saves time – the preparation of a 200 mL surrogate mixture takes less than 5 minutes
- Lower reagent consumption



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