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Petroleum products — Density versus temperature relationships of current fuels, biofuels and biofuel components

Produits pétroliers — Densité contre température relations des carburants actuels, les biocarburants et leur composants

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation on the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT) see the following URL: www.iso.org/iso/foreword.html.

This document was prepared by ISO/TC 28, *Petroleum and related products, fuels and lubricants from natural or synthetic sources*.

Introduction

The density of hydrocarbon fuels at a standard condition of temperature and pressure is used to define the quantity (standard volume) of the product during trade and fiscal transactions. To ensure standardization in the calculation of standard volume and density from actual conditions the thermal and pressure expansion factors are calculated through the application of standardized methods and algorithms.

In the advent of new fuel compositions like HVO ("Hydrogenated Vegetable Oil") as well as blends with bio products like ethanol and FAME ("Fatty Acid Methyl Esters") in the markets, the question was raised whether the density/temperature relationships, which have been applied for more than 60 years to transform the density or volume of a petroleum product, are a temperature measured at transport time or a "reduced" density or volume value at a standard temperature (15°C and in some areas 60 °F).

In order to identify potential differences for these new products, the German petroleum standardization committee (DIN-FAM) started as early as 2003 to make extensive density/temperature measurements starting with FAME. Examination of additional products followed, and other associations like AFNOR and the Energy Institute (EI) also shared their results of similar investigations.

This document also recommends procedural steps to obtain data which will determine the thermal expansion of new or alternative fuels and blends hence allowing a comparison to accepted and standardized correction factors (e.g. Petroleum Measurement Tables - ISO 91, IP 200 and API MPMS chapters 11.1, 11.2.4 and 11.5).

This document collates the executed measurements, modelling procedures and results in order to keep measured data available for later reference, including some recommendations for further work and a list of possibly unresolved questions.

For a number of reasons the work has been restricted to fuels, bio fuel components, and their blends and to some burner fuels and components. The majority of these examined products followed European Fuel Specifications such as EN 228, EN 590, EN 14214, EN 15376, and the reference temperature was kept at 15 °C. The work only covers the thermal expansion of the products at a standard condition of pressure and has not been extended to compressibility.

This document also recommends procedural steps to obtain data which allows a decision to be made on whether any completely new fuel composition can or cannot use the published internationally accepted API Petroleum Measurement Tables ("PMT") which are also the basis of several international and national petroleum measurement standards.

In addition, this document contains an extensive list of publications which can yield further in-depth information about this complex and interesting petroleum measurement topic.

Petroleum products — Density versus temperature relationships of current fuels, biofuels and biofuel components

1 Scope

This document lists and describes recent density measurements at different temperatures for biofuel components and biofuel blends such as gasoline E5, E10, E85 and biodiesel B100, B7, as well as domestic heating oils and paraffinic diesel fuels.

It can be used to calculate <alpha15>, the thermal expansion coefficient from a given temperature to 15 °C. This document can also serve to compare several aspects of density/temperature modelling and to check for compliance with and limitations in relation to existing calibration requirements. It can help in the determination of specific necessities for the grouping of fuels into common product family classes, also suggesting ways to treat fuels or components with an unusual behaviour. In addition, this document proposes possible steps for an internationally harmonized handling of new components coming into the market.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

No terms and definitions are listed in this document.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

4 Summary

Several extensive sample sets comprising artificial blends as well as market fuels were analysed with respect to their temperature-dependent densities. The purpose of these analyses was to find out if the density, as well as the volume, at a certain temperature can be predicted using the constants, group constants and regression models of the internationally used API Petroleum Measurement Tables (PMT) published in 1960 and revised in 1980[13].

The examined products were:

— diesel fuels (B0, B5, B7) according to the European standard fuel specification EN 590[28], supplemented by some additional blends with FAME;

— fatty acid methyl esters (biodiesel) of different compositions and origins which are in the market today[31];

— petrol (E0, E5, E10) according to the European standard fuel specification EN 228[27], supplemented by some additional blends with ethanol up to E100;

— domestic heating fuels according to DIN 51603-1[29], also as low sulfur grade;

— several samples of paraffinic diesel fuels (GTL, XTL) for which an European standard fuel specification is established as EN 15940[30].

The main intention of this study was to find out if individually calculated thermal expansion coefficients α_{15} and their corresponding densities (or volumes) at 15 °C are close enough to the values predicted by the published PMT values, taking into consideration the precision requirements of the EC Measuring Instruments Directive. This directive is of particular importance e.g. for the calibration of volume metering equipment.

The executed studies indicate that although some small biases were found in most cases, the predictions described in the PMT may still be used, except for a smaller number of cases being:

— MD/diesel blends with more than about 50 %(*V/V*) of coconut methyl ester (CME);

— automotive E85 fuels with more than about 40 %(*V/V*) ethanol content;

— some new products like paraffinic diesel fuel.

Since it not possible to extrapolate such findings to any other kind of new product types, a recommendation is given to investigate such temperature versus density/volume behaviour when new fuel specifications are under development.

In any case it is strongly recommended to decide before any such investigation if the resulting model should be just good enough to fulfil the requirement or if best possible precision is wanted. This decision can have some influence about the choice of the best suited regression model.

As a long term perspective, a full revision of the PMT models and constants should be considered especially if it is expected that there will be much more variation in fuel composition as compared to the last, say 50 years.

5 Background and motivation

It is common knowledge that the density of a product in its liquid phase depends mainly on product composition; temperature, due to extra- and intermolecular motion.

In addition, pressure can also affect density, but this effect was not investigated here because the changes caused by pressure are orders of magnitude smaller than those from temperature changes.

For trading and transport, the density-temperature function of a product is a very important product property for the determination of the product amount because the temperature of a liquid fuel can be as high as 50 °C, whereas, e.g. for tax reasons, almost all regulatory requirements demand that product densities are reported at a standard temperature of 15 °C (or, like in the US, also at 60 °F) as a prediction using these density-temperature procedures.

The internationally accepted procedures for the determination and application of density and volume transformation from one temperature to another or to a standard temperature have been developed and standardized by the API and ASTM and are commonly referred to as the Petroleum Measurement Tables (PMT). These tables have been adopted by ISO (ISO 91) and by OIML by referring to ISO 91[14].

The tables and the procedures within them have been have been applied successfully and with satisfactory precision for more than 60 to 70 years and provide a standardized and accepted basis for trade[1][2][3][4].

NOTE 1 This report refers to the three latest version of the API tables, published in 1960, 1980 and 2000. The version from 2000 is a computer adoption of the 1980 version, including pressure correction.

It is evident that this success is mainly based on the existence of comparatively small compositional changes across a specific product family. The advent of biofuels and biofuel components like FAME (Fatty Acid Methyl Esters) in the market raised the question of whether the PMT tables could still be applied with acceptable precision for the predicted density at reference temperature. This question

led to several series of FAME density measurements at different institutions in Germany, the UK and France, and probably also in many other countries.

Later this campaign was extended to ethanol, petrol blends (E0, E5, E10, … E85, E100) and to several other products like Hydrogenated Vegetable Oil (HVO), paraffinic Diesel fuels (GTL, XTL).

NOTE 2 Most of the mentioned calculations and procedures and their background are documented at least in part in the available standards, publications and regulatory documents, so a large portion of the described detail is supposed to be common knowledge for the experts working with petroleum measurement regularly. It is the intention of this document to describe everything to such a degree of detail that also people new to this field of expertise have a chance to follow and understand all of the contained reasoning.

Although the latest version of the PMT and ISO 91 are recommended, older versions are sometimes still employed as defined in local regulation, practice or commercial agreements.

These facts might be able to explain some differences which could not be explained otherwise.

6 Basic analytical considerations

6.1 Intentions of this document

In order to fully comprehend the discussions and arguments presented in this document, the following clauses set out the relevant definitions, procedures, facts, calculations and consequences.

It is not the intention of this document to copy already existing content from other existing publications or standards, but it was found essential to compile all relevant facts in one place. For further information, see the Bibliography.

6.2 Physical property density

The physical property density is defined as the ratio of mass over volume as shown in Formulae (1) and (2). It is important to note that the density depends to a large extent on the product temperature such that with increasing temperature density decreases (volume increase e.g. due to more molecular motion) while mass remains constant. As this document only deals with (liquid) fuels, phase transitions to the gaseous or solid state are not discussed. Such transitions can become a problem at extreme product temperatures.

NOTE 1 While density is normally represented by the Greek letter ρ, this document uses a capital D for density for easier and more clear writing. Further information is often added as an index or given in brackets. This means that e.g. $D15$ and $D(15)$ will mean the same thing:

$$\rho_t = m / V_t \quad (1) \quad \rho_t = m^* V_t \tag{1}$$

$$D(t) = m / V(t) \tag{2}$$

where

ρ, D is the sample density; usually in g/ml or kg/m^3;

m is the sample mass (NOT the weight); usually in g or kg;

V is the sample volume; usually in ml or m^3;

t is the sample's temperature; usually in °C.

The numerator of the density definition is mass and not, as sometimes wrongly stated, weight, which is the property when gravity acts on the mass of a product. Therefore, constructs like density in air or density in vacuum simply do not exist. For cases where weight is required, a correction for the air buoyancy mass can be applied.

NOTE 2 There are several incarnations of a reported density value, depending on the fact if this value was obtained by direct measurement at the required temperature; or if it was predicted from measurement at a different temperature using PMT procedures for appropriate conversion to standard temperature. In cases where this can become relevant, corresponding mention is made in this document.

NOTE 3 There are several test methods, all using different physical principles for the determination of the density of petroleum products/fuels (see experimental section). Only the quartz oscillator test method has been used in this report as prescribed in ISO 12185. This is currently the most used density test method for liquid fuels.

6.3 Density for (defined) product blends/mixtures

For many product blends density follows a linear regime, i.e. the density/volume of the blend has a linear relationship with the volumes and densities of the components when measured at the same temperature.

However exceptions to this rule are known from literature and recent work which show that for blends of some components the relationship can be far from linear. Examples include:

— temperature of mixture changes during blending;

— molecular and compositional structures of blend components are significantly different;

— other physical effects occur such as modified molecular solvent cages e.g. for alcohols (OH bonding).

6.4 The volume correction factor (VCF)

The definition for the volume correction factor (VCF) is given in Formulae (3) and (4). The VCF is simply the ratio of density at the temperature t of interest over density at standard temperature (normally 15 °C). It is therefore the basic proportionality function for the calculation (prediction) of density (or volume) at standard temperature from a density (or volume) measured at another temperature t or vice versa. Elaborate models like the PMT and several others have been developed for construction of this VCF function for single products as well as for commonly used product families. The following sections of this document will give more detail about these models and their modelling strategies. But first we should have a look at the basic definitions.

$$\mathrm{VCF}(t,\mathrm{ref}\cdot t)=D(t)/D(\mathrm{ref}\cdot t) \tag{3}$$

$$\mathrm{VCF}(t,\mathrm{ref}\cdot t)=V(\mathrm{ref}\cdot t)/V(t) \tag{4}$$

where

VCF being volume/volume or density/density ratios (dimensionless);

D, V being density and volume as explained in Formula (1);

$ref{\cdot}t$ being the sample's reference temperature; usually 15 °C;

t being the sample's temperature; usually in °C.

It is evident that the VCF has the value 1,000 0 at the reference temperature (usually 15 °C). Also, individual VCF(t) functions for different products will by default always intersect at the reference temperature. It is also important to note that each single VCF function has been derived for a specific sample of a product family for limited temperature or density ranges which should not be extrapolated.

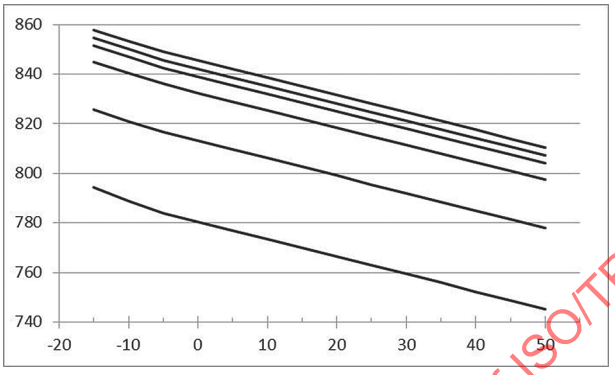
The form of the VCF function can range from nonlinear/exponential, linear, and even constant (like for some products with little variation in composition and density/temperature range). The models used for petroleum metering should reflect such different functional behaviours.

For products of similar/comparable density, temperature and composition, the PMT allow some grouping into product families. Here, a hopefully large and representative number of product family

members is investigated. This investigation results in a set of constants K_0, K_1, K_2, from which the thermal expansion coefficient α_{ref} can be calculated with inclusion of the density at reference temperature (see modelling section for more detail).

6.5 Graphical representations of the density/temperature behaviour

Figure 1 shows a commonly used and typical graphical representation of the $D(t)$ behaviour for a selection of six gas oils.

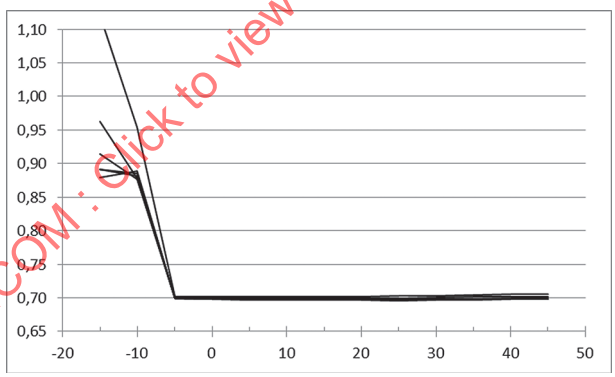


Key

X temperature in °C

Y density change in kg/m3 per °C

Figure 1 — Density/temperature function



Key

X temperature in °C

Y density in kg/m3

Figure 2 — K_0E/temperature function

The graphs display a number of issues to remember.

— Densities for members of one product family can stretch over a large range.

— The slopes for members of a product family are often very similar (but not necessarily identical (depending on the required prediction quality).

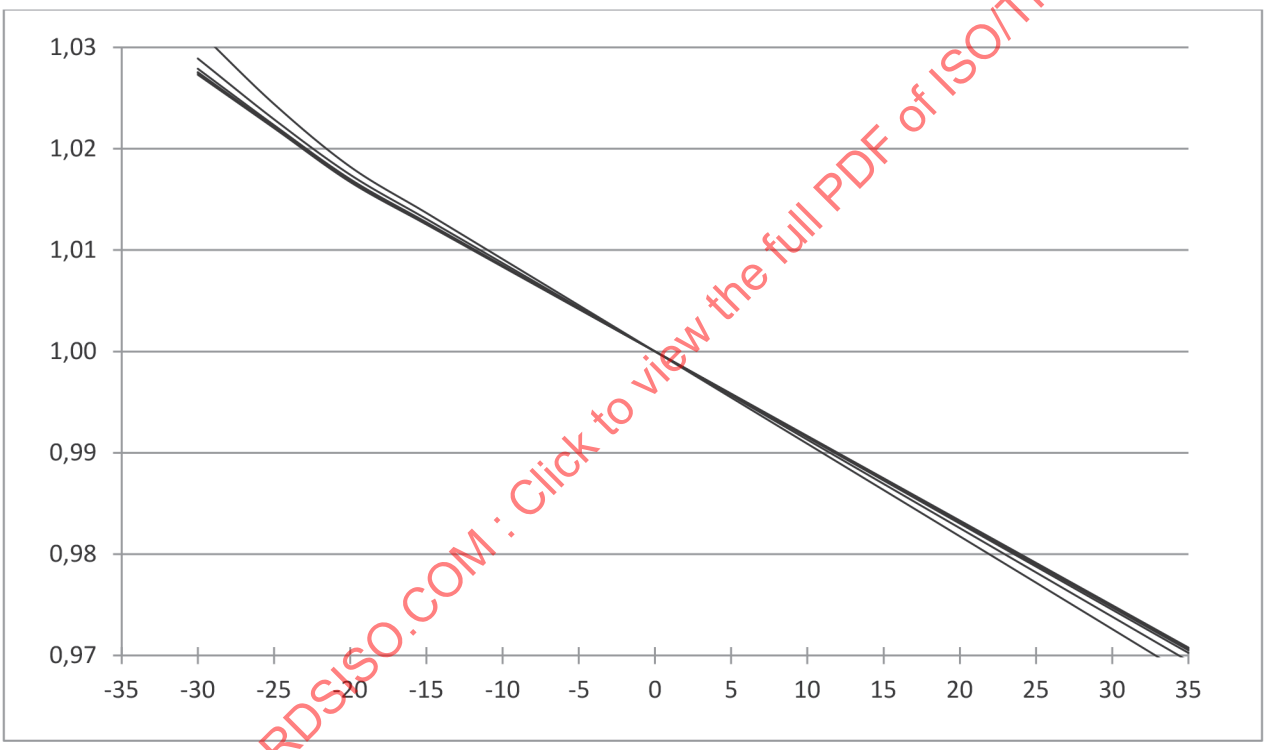
— From a superficial viewpoint, the $D(t)$ curves seem to be (almost) linear. However, this can be quite different for other product families. Therefore, a nonlinear (exponential) modelling approach has been (and still is) used traditionally in the international PMT community.

Figure 2 indicates that the temperature range for the $D(t)$ modelling can also be quite important. The displayed case for six gas oils suggests that irregular behaviour can occur at lower temperatures where there is a good chance of crystal formation or even solidification. A model has to consider these phase transition effects when a reliable and most precise prediction is wanted (same is true for extreme high temperatures (bubbles, evaporation, boiling).

Current experience from field transport experts suggest that for the petrol, diesel and biofuels investigated in this document, a temperature range of about −5 °C to about 50 °C is usually sufficient.

Figure 3 displays the VCF(t) plot for the same six gas oils. At $X = 0$ (i.e. at standard temperature of 15 °C) all curves intersect in the same point (at y = 1,00) by definition, and potential differences between product family members become more visible the farther the temperature is away from the standard temperature.

NOTE The VCF(t) curve shown in Figure 3 is simply constructed by division of each $D(t)$ value by the sample's reference $D(15)$ value. These curves do not represent the results from the PMT procedures, for which the use of a specific PMT regression model is assumed. Nevertheless, the plot shows nicely the similarities and differences between similar samples of one gasoil family.



Key

X (t−15) in °C

Y VCF(t,15)

Figure 3 — *VCF*(t,15) plot for the same six gasoil samples

7 Applicable VCF models

7.1 General

Several models have been developed over the years for petroleum measurement of diverse petroleum products. For an in-depth sight and some important history, see the Bibliography. Since the focus of

this document is on fuels, bio fuels and their components (i.e. Tables B of the petroleum measurement tables), the list of useful and common models is reduced to the following:

— exponential model — the mainly used model in the PMT for fuels of group B;

— linear models — a simplified model derived from the exponential model;

— constant value model — promoted by some government chemist associations.

Other sometimes proposed models like third order parabolic regression do not, at least in Europe, play any important role in the trading of conventional and bio-based fuels and their components.

7.2 Exponential model (for a single sample)

Used and published in the PMT, it represents clearly the most often applied and internationally accepted VCF model. The definition is given in Formula (5). The two constants α_{15} and K describe the slope and curvature of the VCF function. For all fuel related products of mineral oil group B, a fixed valued of K = 0,8 has emerged over the years and is still used in the PMT. The development of group family constants for α_{15} is explained in the next clause.

$$\mathrm{VCF} = \exp\left(-\alpha_{15} * dt * \left(1 - K * \alpha_{15} * dt\right)\right) \tag{5}$$

where

α_{15} is the thermal expansion coefficient at reference temperature (normally 15 °C, but some countries also use 60F as ref. temperature, in which case α is given as α_{60F});

K is a constant describing the curvature. Normally this value is always fixed at K = 0,8;

dt is the difference between measured and reference temperature (normally 15 °C).

The α_{15} is calculated and used for only the specific sample for which at minimum 10 densities at different temperatures have been measured. This temperature range should include the temperatures of interest used during transport, but some care should be taken at extreme temperatures to avoid solidification or bubbling in the sample. These measured data pairs $D(t)$ and t are then submitted to a regression procedure specified in API MPMS Chapter 11.1. Annex A contains a script using the public domain statistical scripting language R, which may be used for the determination of α_{15}.

IMPORTANT — It should be noticed that the 60 °F reference temperature equals to 15,666 67 °C (i.e. 15 °C = 59 °F and not 60 °F), and that in the PMT, given α_{15} values are in reality values for 15,666 67 °C. It is an obvious international agreement to ignore this difference for "α" because the slopes at 15 °C and 15,666 67 °C should be quite similar. To avoid any doubts, this TR will give D(15), D(60 °F), α_{15} and $\alpha_{60\ °F}$ wherever possible. The difference between D(15 °C) and D(6 °F) can amount to more than 0,5 kg/m³. This should be considered when precision issues are discussed.

NOTE DIN 51757[17] has a section for pure petrochemical products (demonstrated Y-Table), for which also different values for K have been developed which to minimize the residuals between measured and predicted values. More information, including some example data, about this Y-table is given in Annex B.

7.3 The linear VCF model

The linear VCF model can best be described as a derivative/simplification of the exponential model via a Taylor series as described in Formula (6) – simplification 1) and Formula (7) – simplification 2). It may be used when curvature of the VCF function is minimal and when differences between linear and exponential model are tolerably small.

$$\mathrm{VCF} = 1 - \alpha_{\mathrm{ref}} * dt - 0{,}3 * \alpha_{\mathrm{ref}}^2 * dt \tag{6}$$

$$\mathrm{VCF} = 1 - \alpha_{\mathrm{ref}} * dt \tag{7}$$

Introducing the densities from the VCF definition then leads to:

$$D(t) = D(15) * (1 - \alpha_{15} * dt) \tag{8a}$$

$$\text{or } V(15) = V(t) * (1 - \alpha_{15} * dt) \tag{8b}$$

where

VCF is the volume correction factor for temperature t;

$D(t)$ is the density at temperature t;

$D(15)$ is the density at the reference temperature (15 °C);

α_{ref} is the thermal expansion factor at reference temperature (15 °C);

dt is the temperature difference (t – 15) in °C.

The linear model produces a straight line, forfeiting the chance to detect and incorporate any nonlinear behaviour of the VCF-function. One well-noticed advantage is that the needed regression for the detection of α_{15} from minimal 10 density/temperature pairs can be done with any regular regression function like those provided by Excel or other off the shelf statistical software.

As will be shown in the experimental section, this linear model can be applied to FAME, where the thermal expansion coefficients do not vary so very much over the FAMES' density ranges, but it is strongly recommended to check the residuals and compare them with those from the exponential models before decisions to use the linear model are made.

It is important to notice that, just like for the exponential model, the regression result α_{15} is in principle only valid for the examined sample. There is not much procedural documentation about how to arrive at a (possibly $D(15)$ independent) "α_{15}" group product family value like they can be found in the literature and published standards for petrol.

A variation of the Linear Model is also applied in the European FAME specification, EN 14214,[31] as specified in Formula (9). The slope of 0,723, and a mean density of $D(15)$ = 886,3 kg/m^3, averaged over seven different FAME samples has been developed in a research project lead by J. Rathbauer[9].

$$D(15\ °\mathrm{C}) = D(t) + 0{,}723 * (t - 15) \tag{9}$$

7.4 The constant value model for a specific product family

This model is best explained by Formula (10). It is mainly promoted by the metrology institutes, such as PTB (Physikalisch-Technische Bundesanstalt, German Metrology Institute), for the calibration of volume meters, taking into consideration the allowable prediction tolerance of max. ±0,2 % as specified in the EC machine directive.

Other than using a still density/sample dependent thermal expansion coefficient α_{15} like in the exponential and linear model, a mean slope k_{0E} is used obtained from the slopes of a number of samples from the product family under examination. Values for k_{0E} are generally prescribed in regulations for volume meter calibrations. For more details about this model see [10]. Figure 4 shows some k_{0E} values

suggested by the PTB (German government chemist) for commonly traded products. It should be noted that these averaged k_{0E} values do no longer depend on the sample's density.

$$\mathrm{VCF} = \frac{D(t)}{D(15)} = \frac{V(15)}{V(t)} = 1 - k_{0E} * (t - 15) \tag{10}$$

The maximum temperature difference of 35 °C and the precision requirement of maximum ±0,2 % then leads to a permissible tolerance band of $|\Delta k| \leq 5 * 10^{-5}$. Individual slopes k from which the mean k_{0E} is calculated have to fall inside the range ($k \pm \Delta k$), otherwise the average value model cannot use the prescribed k_{0E} for that particular product or sample.

This is also reflected by the fact that e.g. in Germany, the k_{0E} values have been updated in different editions of the volume meter calibration regulations (see e.g. Figure 4) along with several product composition changes over the years. It is also important to note that this mean k_{0E} is not influenced by the product reference density as will be shown is the case to the PMT exponential model.

Table 1 — k_{0E}-values for the constant value model as promoted by the PTB

Product group	Date of PTB publication	k_{0E} (1/K)	$\pm\Delta k$ (in 1/K) for Δt = 35 °C	Remarks
Group B,1	2004	$1{,}21 * 10^{-3}$	$5 * 10^{-5}$	For E0,E10, E80, E100
Group B,3 and B,4	2004	$0{,}84 * 10^{-3}$	$5 * 10^{-5}$	For Diesel, FAME (RME and SME) and Heating oil (HEL)
Group B,3 and B,4	2011	$0{,}84 * 10^{-3}$	$5 * 10^{-5}$	For Diesel, HEL, CME from B0 to B40
Group B,1 - petrol	2011	$1{,}27 * 10^{-3}$	$5 * 10^{-5}$	For E0 .. E40
Group B,1 - ethanol	2011	$1{,}14 * 10^{-3}$	$5 * 10^{-5}$	For E60 .. E100

Some additional aspects concerning the constant volume model should get some special attention:

— the major use is for the calibration of volume meters as prescribed by (e.g. national) regulators;

— use of a specific k_{0E} value can only cover a small variety of samples inside just one product family, and when there is too much variation in product composition or slopes of the $D(t)$ curves, the constant value model could no longer comply to the pre-set precision requirements;

— the constant value model is, of course, easy to use, but also using up most of the permissible measurement uncertainty, leaving little to no room for other measurement uncertainties like those coming from the determination of density and temperature. In the analytical community, this is sometimes seen as a contrast to the wish for best possible precision in the modelling of results.

NOTE Since this document does not intend to interfere with any regulated issues, the constant value model is not discussed any further here.

8 Developing the group constants K_0, K_1, K_2 for the PMT Group B products (see Table 1)

In the previous clauses we have described the development α_{15} and $D(15)$ for just one product. Much effort has been put into the measurement of these values for the different product families over the past decades to determine some sort of common model for a complete product family. ASTM and IP, for example, explain such measurements and additional regression work from several hundred product family members in their standards, and indeed, a useable and rather robust regression model for the

group B product family has been established, as described in Formula (11). This regression model is still in use today and has been the reference PMT routine for many decades.

$$\alpha_{15} = K_0 / D_{15}^2 + K_1 / D_{15} + K_2 \tag{11}$$

Table 2 presents the corresponding values for α_{15}, $D(15)$ and the regression constants K_0, K_1, K_2 for the individual members of the PMT Group B Products.

Table 2 — Group constants for PMT Group B product family

	Petrol		Naphtha		Jet/Kerosene		Fuel Oil	
Const.	K_0	346,422 80	K_0	2 680,320 6	K_0	594,541 80	K_0	186,969 60
Const,	K_1	0,438 80	K_1	0,000 00	K_1	0,000 00	K_1	0,486 20
Const,	K_2	0,000 00	K_2	−0,003 363 12	K_2	0,000 00	K_2	0,000 0
$D(15)$	Lo	600,0	Lo	770,5	Lo	787,6	Lo	838,6
$D(15)$	Hi	770,4	Hi	787,5	Hi	838,8	Hi	1 200,0

NOTE 1 In some older publications and regulations, regression constants A and B have been used in the case of naphtha instead of K_0 and K_1. Constant K_2 could then be deleted which was quite important in earlier times when computer memory was sparse.

This so-called $\alpha_{15}/D(15)$ data space is in use for more than 50 years now. It also constitutes an international reference for the Petroleum Measurement of fuels. The graph in Figure 4 shows clearly four adjacent different sections, and Table 3 explains that, for example, EC fuel specifications cover only parts of the whole density/α_{15} range. It is also easy to recognize that PMT product $D(15)$ limits are not identical with the limits from the EC fuel specifications, as e.g. Diesel fuel spans over parts of jet/kerosene and fuel oil.

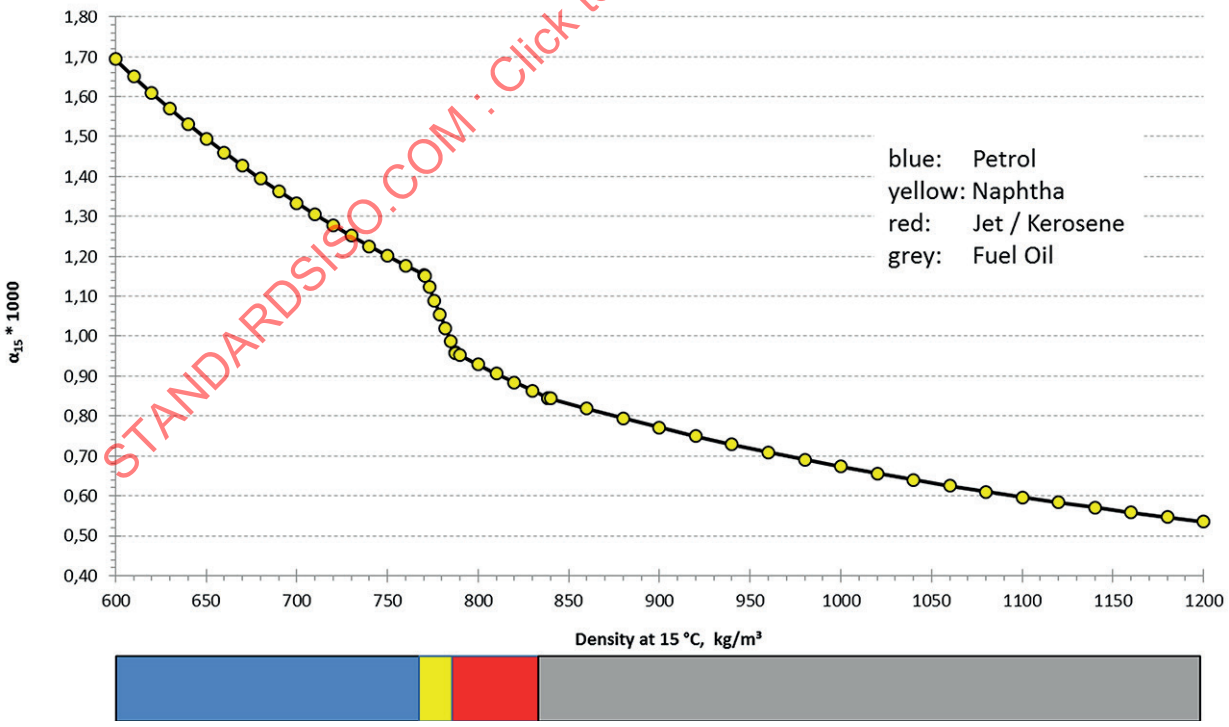


Figure 4 — Graphical display of the $\alpha 15$ <> $D(15)$ PMT model for Group B products

Table 3 — density ranges from EC Fuel specifications

		Petrol (EN 228)		**Diesel** (EN 590)		**FAME** (EN 14214)
$D(15)$	Lo	720,0	Lo	820,0	Lo	860,0
$D(15)$	Hi	775,0	Hi	845,0	Hi	900,0

NOTE 2 The graphical representation is simply the regression function for several hundred "conventional" fuel samples (dissected into four groups, see Figure 4), where the individual points [$D(15)$,α_{15}] will lie a bit above or below the regression function. Since the original data point from which the models have been developed were not available for this project work, only some summary statements to be found in the ASTM and API papers are available for judging how well the individual group family members fit into the models.

Although the original data points used for setting up the regression are quite old, ASTM D 1250 and API both explain some more detail about the quality of this regression which is working surprisingly well considering all the changes to product compositions over the last, say 30 years (sulfur, aromatics, boiling range, etc.).

The general task for the experimental work executed in this document was to find out if these conventional group constants would also be applicable to more and more appearing new products and components like paraffinic fractions, bio fuels and components thereof, ethanol HVO, FAME and others. In order to allow such a judgement, one more regulatory requirement from the EC Measuring Instruments Directive[16] should be considered, which is described in the next clause.

IMPORTANT — From a closer inspection of Formula (11) it is easy to conclude that the calculation is straight forward when the density at 15 °C is known, i.e. when the final target of the exercise is the prediction of density or volume at some higher or lower temperature.

For the reverse case, i.e. when the starting temperature t is not 15 °C, the calculation is iterative and a bit more laborious:

— first, select and assume a starting density at 15 °C, D(15,test);

— then calculate the corresponding α15, test plus the corresponding $VCF_{test}(t,15)$;

— then calculate the resulting $D(t,test)$ and compare this with $D(t,measured)$;

— if there is a match, the needed $D(15)$ for the final calculation of α_{15} has been found;

— in case of a missing match, iterate with a somewhat altered starting density D(15,test).

9 European precision requirements for volume meters revisited

The European Measurement Instrument Directive[16] - Annex MI - requires that the prediction error made during petroleum metering should satisfy Formulae (12a) to (12d), meaning that the modelling error should be less than 0,2 %; in other regions of the world similar regulations might apply. A very first and quick check would be to measure D(50 °C) and then use the PMT procedures to obtain D(15 °C, predicted) which then should be compared to check if the ratio $R = D$(15 °C, predicted)/D(15 °C, measured) falls into the range (0,998 < R < 1,002). If this condition is met, there is a very good chance that the conventional PMT may be used without problems. This approach, however, incorporates the measurement uncertainty for the density measurement in combination with the modelling error. Therefore, a more reliable procedure uses the VCF to make some judgement for the applicability as follows:

The precision questions about the applicability of the PMT model transforms into the question if the individual thermal expansion coefficient $\alpha_{15,i}$ for product (i) and, also considering dt, it is sufficiently close to the "predicted" value from the conventional model. Some algebra then leads to the set of Formulae (13a) to (13d).

$$\mathrm{VCF}(\alpha_1;dt)=\exp\left(-\alpha_1 * dt - 0{,}8 * \alpha_1^2 * dt^2\right) \tag{12a}$$

$$\mathrm{VCF}(\alpha_2;dt)=\exp\left(-\alpha_2 * dt - 0{,}8 * \alpha_2^2 * dt^2\right) \tag{12b}$$

$$\left(1+\frac{X}{100}\right) \geq \mathrm{VCF}(\alpha_2,dt)/\mathrm{VCF}(\alpha_1,dt) \geq \left(1-\frac{X}{100}\right) \text{ with } X = 0{,}2 \tag{12c}$$

Solving Formula (12)c) for α_2 then gives (12d) which allows to calculate the max./min. allowable α_2 to give the maximum difference to the model-derived α_1 without violating the precision limit X. For this type of consideration, a dt of max. 35 °C is most often used.

$$\alpha_2 \geq \left(\sqrt{\alpha_1^2 + \frac{\alpha_1}{0{,}8 \cdot dT} - \frac{\ln(1 \pm X/100)}{0{,}8 \cdot dT} + \frac{1}{1{,}6^2 \cdot dT^2}}\right) - \frac{1}{1{,}6 \cdot dT} \tag{12d}$$

As Formula (12)d) indicates, the maximum allowable prediction corridor for the thermal expansion coefficient is getting smaller with growing temperature difference dt, proposing that when the given precision requirements are fulfilled at higher temperature differences, this will also be true for some smaller dt. Figure 5 gives a first impression of allowable corridors for α_{15} for the prediction errors in the four PMT Group B product family. We have used three precision levels (0,1 %, 0,2 % and 0,3 %) in order to allow some sort of quantitative graphical display for the [D(15); α_{15}] coordinates of a new product type.

NOTE 1 This second checking procedure has been used for all measured samples and new components. It is therefore easy to show corresponding plots how good (or bad) the examined data point fits into the corresponding conventional model.

NOTE 2 Other regulatory regimes can have similar requirements. The use of the European requirements is given as illustrative of the methods and expectations.

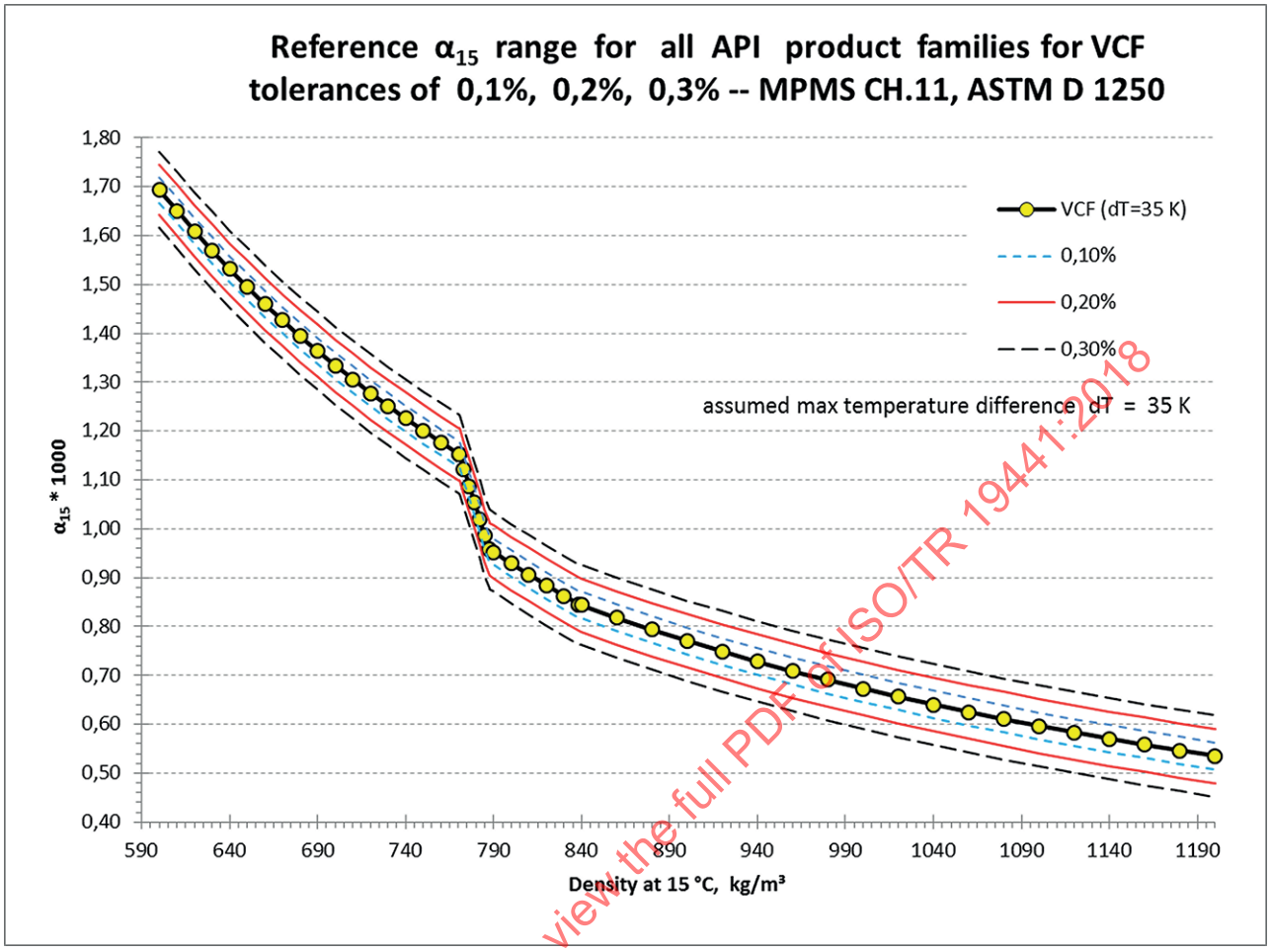


Figure 5 — Allowable precision corridors for individual α_{15} values

10 Experimental details concerning the density measurement

10.1 Choice of density determination method

Several internationally well-known test methods are in use for the density determination for petroleum and related products. The most often used ones for the fuels of PMT Group B are:

a) ISO 3675.

b) ISO 12185.

Only ISO 12185 has been used in the experimental work described in this document, simply because we could find more volunteers using the Quartz U-tube than we could for the hydrometer method.

The U-tube oscillator test equipment is well described in many standards and publications, so the measurement principles do not need further elaboration. Suffice to say that several test equipment generations are in use, allowing a read-out from 1 to 3 decimal places (units given in kg/m^3). PTB, where a larger number of samples have been measured, claims a measurement uncertainty for their instrument of less than 0,005 kg/m^3.

It is important to notice that basically all test equipment also with lesser decimal digits allow to execute the calculations and routines as specified in the petroleum measurement standards, considering the fact that most data points and product family group constants which have been developed decades ago with somewhat less performing test equipment are still used today.

It is also worth mentioning that almost all today's test equipment has built-in PMT routines, such that it is seldom known if a reported value is a real measured one or if it is the result of a PMT calculation.

ISO 12185 is also bit sparse about precision information for repeatability, *r*, and reproducibility, *R*, for different product types and, more important, for different measurement temperatures. Some results especially for FAME from earlier round robin exercises at DIN-FAM are given in Annex C.

NOTE 1 Because the original precision statements in ISO 12185 were based on models of meter that are generally no longer in use, a Round Robin is being organized by ISO TC 28/SC 2, under the auspices of the UK Energy Institute.

NOTE 2 A possibly important issue which was observed, can be the readout of the density before the temperature in the measurement cell has reached a stable state. Newer instruments with more advanced controls can help avoiding these "hasty" measurements. However, it is still important to take care as this safety function can be overridden in many cases.

NOTE 3 In contrast to many other publications it was found necessary to list all measured data points for potential later reference in Annex D, together with the results. Some other papers just reference documents in the internet, but many of these links are by now broken so that data are no longer easily available.

10.2 Participating laboratories

A large number of industry laboratories from the petroleum and automobile industry, independent laboratories, laboratories from the German customs offices and from the German government chemist (PTB) have made significant contributions. Some of the PTB measurements were uploaded to the internet (look for PTB petroleum measurement).

Almost all of these laboratories are accredited for petroleum test methods, participate in petroleum standardization activities of DIN-FAM and CEN/TC 19 and participate in round robin tests for petroleum products. All laboratories have a long term experience with density/volume measurement and metering procedures.

10.3 Samples

The tested samples set comprised:

— FAMES, mainly RME, SME (Soy), PME (Palm), CME (coconut) and some others with different compositions taken from filling stations (B100 qualities) or from main production lines, fulfilling the EC specification EN 14214;

— diesel fuels taken from filling stations and from different main production lines fulfilling EN 590;

— petrol from filling stations and from different main production lines fulfilling EN 228;

— domestic heating oil (HEL) and low sulfur domestic heating oil fulfilling DIN 51504;

— ethanol samples from main production lines fulfilling EN 15376;

— several other new products components line paraffinic diesel (GTL), etc.;

— several volumetric blends have been prepared from these samples in order to fill a few gaps in the data space.

10.4 Measurement ranges

Density measurements were conducted at a minimum of 10 or more different equidistant temperatures if possible (e.g. each 5K apart) for an overall product related range as depicted in the diverse tables of measurement results. The difference between two adjacent temperatures then can give a first indication about how monotonic curvature of the $D(t) = F(t)$ function is.

In this context it has been observed that for mostly middle distillate products, some irregular behaviour can occur at lower temperatures about 0 °C and below. This seems to indicate beginning solidification, start of crystal formation or other effects of phase transitions. It such cases, the calculation of α_{15} was done using only the monotonous part of the $D(t)$ curve.

NOTE Most $D(t)$ curves with some degree of curvature can produce slightly different values for $\alpha 15$ and $D(15)$, depending on the lowest temperature used in the PMT regression. So the start and end point of the applied temperature range can indeed make a difference to the resulting α_{15} and $D(15)$ values. See some of them tables for more detail.

FAME experts have soon found out that curvature of the α_{15} and $D(15)$ function is rather linear. For this reason instead of using a temperature range of −30 °C to 50 °C a much smaller range using only four different temperatures (10 °C, 15 °C, 25 °C, 40 °C) can be sufficient to apply the linear model calculation as described in Formulae (7) and (8). Problems with e.g. solidification of the sample in the test equipment can be avoided using this approach.

10.5 First impressions on necessary precision for the $D(t)$ measurement

The possible errors occurring during the application of petroleum measurement procedures can have several different sources.

— Errors from the test method itself in form of repeatability, r and reproducibility, R. The current standard ISO 12185, for example, specifies a reproducibility R = 0,5 kg/m^3 for one product group and an R = 1,5 kg/m^3 for a second product family. Precision values valid for other temperatures are so far also not reflected in the available standards.

— Errors from rounding (i.e. different decimal digits in the density measurement equipment). This error can be regarded as sufficiently small (assuming no systematic bias):

  — 3 decimal digits → 800,001/800,000 → 0,000 1 %;

  — 2 decimal digits → 800,01/800,00 → 0,001 3 %;

  — 1 decimal digit → 800,1/800,0 → 0,012 5 %.

  This short overview explains that reporting decimal places will not have gross impact on the precision of results.

— Temperature control: this was found to be a potential problem if readings could be made before the temperature had reached a stable level. Today, newer instruments usually allow for the readout only when the desired temperature has been reached, however, in many cases this safety measure can be overridden so that still care has to be taken. PTB reports their measurement temperatures to the nearest 0,001 °C, and for practical purposes, the temperature values used in the calculations of this TR have been rounded to the nearest 0,01 °C.

— Modelling errors from the “lack of fit” when samples of differing compositions are combined into only one model; this error is hard to assess, because the old measured data points which have finally lead to the group constants in the published PMT seem to be no longer available.

— Difficulties with unnoticed effects like solidification, crystal formation, or build-up of bubbles. This seems to be a somewhat new observation not extensively discussed in former times.

In the discussions around this project it became soon clear that combined measurement errors do occur and that the largest deviation from the prediction function for α_{15} and $D(15)$ will originate predominantly from the compositional variances in the samples which have been collated into one singular model for a specific product family. This then leads to the conclusion that the most important factors for the construction of stable and reliable models are dominated by the fact of how complete and representative the selected samples used for model building have been.

10.6 Further experimental steps

For each sample, the individual thermal expansion coefficient α_{15} and the related $D(15\ °C)$ was calculated according to the regression procedure (Method C) of API MPMS Chapter 11 (see R-script in Annex A).

The individual data points [$D(15\ °C)$; α_{15}] were then compared against the for α_{15} and $D(15\ °C)$ results obtained by using the conventional published PMT product group constants, including their fit to the ±0,2 % prediction error band as required by the EC Measuring Instruments Directive. For more detail see the diverse tables, graphs and explanations in the following sections.

A comparison of the positions of these individual data points in the plot can be the basis for concluding whether or not the conventional PMT model and constants can be used for the $D(t)$ conversions or if some new procedure would have to be established.

11 Density measurement and interpretation of results

11.1 Middle distillates

Usually diesel fuels, kerosene type fuels and domestic heating oil are considered as middle distillate fuels. For many years, however, new fuels from renewable sources (biofuels) and/or synthetic fuels (paraffinic diesel fuels) from various processes appeared on the market, either as pure fuels or as blend components, showing in some cases significantly different physical and chemical properties.

The density/temperature relationships concerning middle distillates also cover FAME, paraffinic diesel fuels and vegetable oils being used as blend component for diesel fuels and domestic heating oil and/or as a substitute for those.

11.2 Studies on FAME and FAME blends

11.2.1 General

Already from the first EC FAME fuel specification standard (EN 14214), a linear $D(t)/D(15)$ prediction model had been specified which was based on some FAME research work presented at the International Conference on standardization and analytics of biodiesel in Vienna[9].

For a first overview about the $D(t)$ behaviour of different FAMES, several experts especially from the FAME and petroleum industries as well as from central customs services in Germany started $D(t)$ measurements at 10 °C, 15 °C, 20 °C and 40 °C, using the linear regression Formulae (7) and (8) for the prediction model. Similar experiments also were conducted at the UK Energy Institute[21], France and Canada. The US based American Petroleum Institute (API) was also contacted asking for sharing their experiences with the new fuels; future collaboration will probably enhance the studies.

During the course of experimental work, more $D(t)$ measurements have been made to allow some comparison with the more general exponential model.

In addition, the German petroleum standardization committee (DIN-FAM) also conducted a precision study for the application of the quartz U-tube oscillator method application to FAME samples. See Annex C for more detail concerning these precision results.

11.2.2 Using the linear model variant

As described earlier in this document, the $D(t)$ behaviour for the FAMES normally used in the EC market can also be described by a linear model as given by Formula 13 [a repeat from Formulae (7) and (8)].

With the precautions to not use the abnormal low temperature $D(t)$ regions and as well also with the selection of an appropriate temperature series, such linear models can work quite well. The selection of

10 °C, 15 °C, 25 °C and 40 °C tested was found to work well several times. The following tables report a set of measurements using this linear approach:

$$D(t) = D(15\ °C) * (1 - \alpha_{15} * \Delta t) \quad (13)$$

where

$D(t)$ and $D(15\ °C)$ are the densities at temperature t or 15 °C;

α_{15} is the thermal expansion coefficient (unit: 1/°C);

Δt is (t–15 °C) in °C.

Using regular off-the shelf linear regression procedures on a series of [$D(t)$; α_{15}] data points then gives the Y-intercept as $D(15\ °C)$ and a slope equalling $-D(15\ °C) * \alpha 15$.

11.2.3 Pure FAMEs

11.2.3.1 FAME campaign 1 in laboratory A

Four different FAMEs were tested in laboratory A at temperatures between 10 °C and 40 °C (Table D.1), resulting in the α-values listed in Table 4.

Table 4 — $D(t)$ at 10 different temperatures on four FAMES from laboratory A

	PMT exponent Model				Linear Model	
	α(60 °F) * 1 000	D(60°F) (kg/m^3)	α(15 °C) * 1 000	D(15 °C) (kg/m^3)	α(15 °C) * 1 000	D(15 °C) (kg/m^3)
1,RME	0,454 94	882,584	0,818 89	882,985	0,822 33	882,986
2,SOY	0,455 59	884,695	0,820 06	885,098	0,823 49	885,099
3,RME	0,455 19	882,351	0,819 34	882,753	0,822 77	882,753
4,RME	0,454 96	882,806	0,818 93	883,208	0,822 36	883,208

The mean "1 000* α_{15}" for this sample set equals 0,822 74, so that the linear model obtained from laboratory A results is:

$$D(t) = D(15\ °C)\ * (1 - 0{,}822\ 74 * 10^{-3} * (t - 15)) \quad (14)$$

11.2.3.2 FAME campaign 2 in laboratory B

NOTE The FAME samples in campaigns 1 and 2 are not identical.

Four different FAMEs were tested in laboratory A at temperatures between 10 °C and 40 °C (Table D.2), resulting in the α-values listed in Table 5.

Table 5 — Results from $D(t)$ measurement in laboratory B for 4 FAMES (duplicate determinations)

	PMT exponent Model				lin. Model		D15 measured	PMT model Diff in %	LIN model Diff in %
	1 000*α15	D(60F)	1 000*α15	D(15C)	1 000*α15	D(15C)			
RME,1a	0,451 32	882,81	0,812 37	883,21	0,815 70	883,21	883,12	0,010	0,010
RME,1b	0,451 31	882,81	0,812 35	883,20	0,815 69	883,20	883,12	0,009	0,010
SOY,1a	0,452 15	884,89	0,813 87	885,29	0,817 24	885,29	885,23	0,006	0,007

Table 5 *(continued)*

	PMT exponent Model				lin. Model		D15 measured	PMT model Diff in %	LIN model Diff in %
	1 000*α15	D(60F)	1 000*α15	D(15C)	1 000*α15	D(15C)			
SOY,1b	0,452 15	884,89	0,813 87	885,29	0,817 24	885,29	885,23	0,006	0,007
RME,3a	0,451 95	882,43	0,813 50	882,83	0,816 84	882,83	882,78	0,005	0,005
RME,3b	0,452 20	882,43	0,813 95	882,83	0,817 30	882,83	882,78	0,006	0,006
RME,4a	0,452 14	882,91	0,813 85	883,31	0,817 20	883,31	883,27	0,005	0,005
RME,4b	0,452 18	882,91	0,813 92	883,31	0,817 27	883,31	883,27	0,005	0,005

The differences between the PMT model C and linear model calculation to the measured D(15) values are very small, and the differences between the exponential and linear model can be ignored at least for these sample sets.

11.2.3.3 FAME campaign 3 in laboratory C

Ten different FAMEs, one B20 and one B30 were tested in Laboratory C at temperatures between 10 °C and 40 °C (Table D.3), resulting in the α-values listed in Table 6.

The results shown in Table 6 are compatible with those obtained from the data from laboratories A and B.

Table 6 — $D(t)$ duplicate measurements for 10 FAMES and 2 diesel fuels for a set of 4 selected temperatures (10 °C, 15 °C, 25 °C, 40 °C) in laboratory 3

	PMT Exponential Model from measurements only at 4 temperatures				Linear Model from 4 temperatures (10 °C, 15 °C, 25 °C, 40 °C)			(D(15,meas) - D(15,pred)) /D(15,meas)	
Sample	1 000 * α(60 °F)	D(60 °F)	1 000 * α(15 °C)	D(15 °C)	1 000 * α(15 °C)	D(15 °C)	measured D(15 °C)	Diff zu PMT Model in %	Diff zu LIN Model in %
FAME,1a	0,454 34	881,78	0,817 81	882,18	0,821 46	882,17	882,17	5.67E-04	–1.29E-14
FAME.1b	0,454 34	881,78	0,817 81	882,18	0,821 46	882,17	882,17	5.67E-04	–1.29E-14
FAME.2a	0,454 33	882,07	0,817 80	882,47	0,821 46	882,46	882,46	1.13E-03	4.86E-04
FAME.2b	0,454 18	882,08	0,817 53	882,48	0,821 18	882,47	882,47	5.67E-04	0.00E+00
FAME.3a	0,454 38	880,83	0,817 88	881,23	0,821 53	881,22	881,22	7.94E-04	2.43E-04
FAME.3b	0,454 58	880,84	0,818 25	881,24	0,821 90	881,23	881,23	7.94E-04	2.43E-04
FAME.4a	0,455 06	881,06	0,819 11	881,46	0,822 77	881,45	881,45	1.13E-03	4.86E-04
FAME.4b	0,455 06	881,07	0,819 10	881,47	0,822 77	881,46	881,46	1.13E-03	4.86E-04
FAME.5a	0,454 44	885,16	0,818 00	885,56	0,821 66	885,55	885,55	7.90E-04	2.42E-04
FAME.5b	0,454 30	885,15	0,817 74	885,55	0,821 39	885,55	885,55	3.39E-04	–2.42E-04
FAME.6a	0,454 13	883,34	0,817 43	883,74	0,821 08	883,73	883,73	7.92E-04	2.42E-04
FAME.6b	0,454 10	883,34	0,817 38	883,74	0,821 03	883,73	883,73	1.13E-03	4.85E-04
FAME.7a	0,492 45	874,21	0,886 41	874,64	0,890 66	874,63	874,63	6.86E-04	–1.30E-14
FAME.7b	0,492 45	874,21	0,886 41	874,64	0,890 66	874,63	874,63	6.86E-04	–1.30E-14
FAME.8a	0,458 03	881,87	0,824 46	882,28	0,828 17	882,27	882,27	5.67E-04	0.00E+00
FAME.8b	0,458 18	881,88	0,824 72	882,28	0,828 43	882,27	882,27	1.13E-03	4.86E-04
FAME.9a	0,454 44	882,68	0,817 99	883,08	0,821 64	883,07	883,07	1.13E-03	4.85E-04
FAME.9b	0,454 47	882,68	0,818 04	883,08	0,821 70	883,07	883,07	7.93E-04	2.43E-04

Table 6 *(continued)*

	PMT Exponential Model from measurements only at 4 temperatures				Linear Model from 4 temperatures (10 °C, 15 °C, 25 °C, 40 °C)			(D(15,meas) - D(15,pred)) /D(15,meas)	
FAME.10a	0,454 21	882,72	0,817 58	883,12	0,821 23	883,11	883,11	1.13E-03	4.85E-04
FAME.10b	0,454 20	882,73	0,817 57	883,13	0,821 22	883,12	883,12	1.13E-03	4.85E-04
B.20 a	0,467 31	840,25	0,841 15	840,65	0,844 99	840,64	840,64	5.95E-04	0.00E+00
B.20 b	0,467 33	840,26	0,841 20	840,65	0,845 04	840,65	840,65	3.57E-04	−2.55E-04
B.30 a	0,465 80	844,51	0,838 44	844,91	0,842 25	844,90	844,90	9.47E-04	2.54E-04
B.30 b	0,466 04	844,53	0,838 86	844,93	0,842 68	844,92	844,92	5.92E-04	0.00E+00

11.2.4 FAME blends with low sulfur domestic heating oils

Blends with low sulfur domestic heating oil containing different shares of FAME were tested (Table D.4). A two variable linear model can also be used for these types of fuels as described by the following equation:

$$D(t) = A + B * (T–15) + C * X \quad (X = \text{FAME Content in } \%(V/V)) \tag{15}$$

where A, B, C are regression constants from the two variable regression, using the input data from Table D.4. The regression constants for this data set are:

A = 842,308 2; B = −0,703 81; C = 0,392 44

$$D(t) = A + B * dT + C * X \text{ (FAME)}$$

A	842,308 2
B	−0,703 81
C	0,392 44

		$D(t)$ in kg/m³					
Temp, (°C)	**(T–15)**	**FAME 0,05** %(V/V)	**FAME 3,0 %(V/V)**	**FAME 5,0** %(V/V)	**FAME 7,0** %(V/V)	**FAME 10,2** %(V/V)	**FAME 20,1** %(V/V)
10,0	−5,0	845,90	847,00	847,80	848,60	849,80	853,80
10,0	−5,0	845,90	847,00	847,80	848,60	849,80	853,70
15,0	0,0	842,30	843,50	844,20	845,00	846,30	850,20
15,0	0,0	842,30	843,50	844,30	845,00	846,30	850,20
25,0	10,0	835,30	836,50	837,20	838,00	839,20	843,20
25,0	10,0	835,30	836,50	837,20	838,00	839,20	843,20
40,0	25,0	824,70	825,90	826,70	827,50	828,70	832,60
40,0	25,0	824,80	825,90	826,70	827,40	828,70	832,60

For the isolated single blends:

Slope	−0,704 05	−0,703 33	−0,703 10	−0,704 05	−0,703 81	−0,704 52
y-intercept	842,343	843,500	844,261	845,043	846,279	850,221
1 000 * α_{15}	0,835 82	0,833 83	0,832 79	0,833 15	0,831 65	0,828 64

$D(t)$ = A + B * dT + C * X (FAME)	A	842,308 2
	B	−0,703 81

For the combined two-variable linear model:

$D(t)$ = 842,308 2 − 0,703 81 * (T–15) + 0,392 44 * X

where

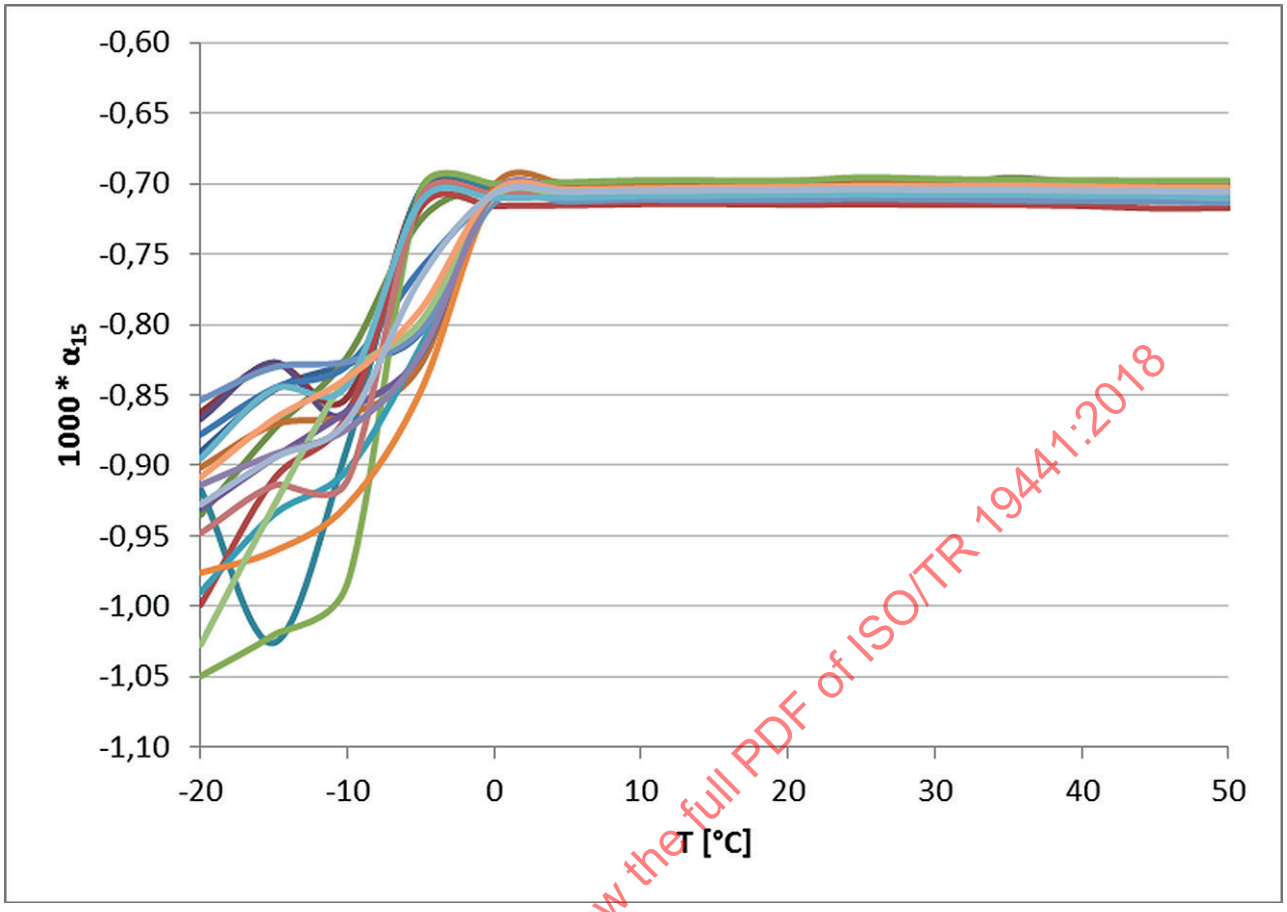
X = FAME Content in %(V/V)

The applicability of this model depends to a large part on the fact that a sufficient number of representative samples and a suitable range of FAME contents (which may not be extrapolated too much) have been included in the modelling process. The structural uncertainty about having met these pre-requirements or not is probably the reason why such models have not found highest possible interest in the testing community.

11.2.5 Market diesel fuels

For the examination of diesel fuels with and without FAME contents, a larger sample set with best possible variation in composition was collected by DGMK and measured by PTB. These samples were collected from almost all German tank farms and refineries. It is therefore assumed that these samples constitute a very representative sample set (one for the summer and one for the winter quality) for the EN 590 diesel fuel specification at least as it can be found in Germany.

The temperature range applied for both the summer and winter qualities was from −25 °C up to 50 °C, and, as discussed earlier, the data reported in Tables D.5 and D.6 and Figures 6 and 7 display the already mentioned abnormal $D(t)$ slopes/curvatures.

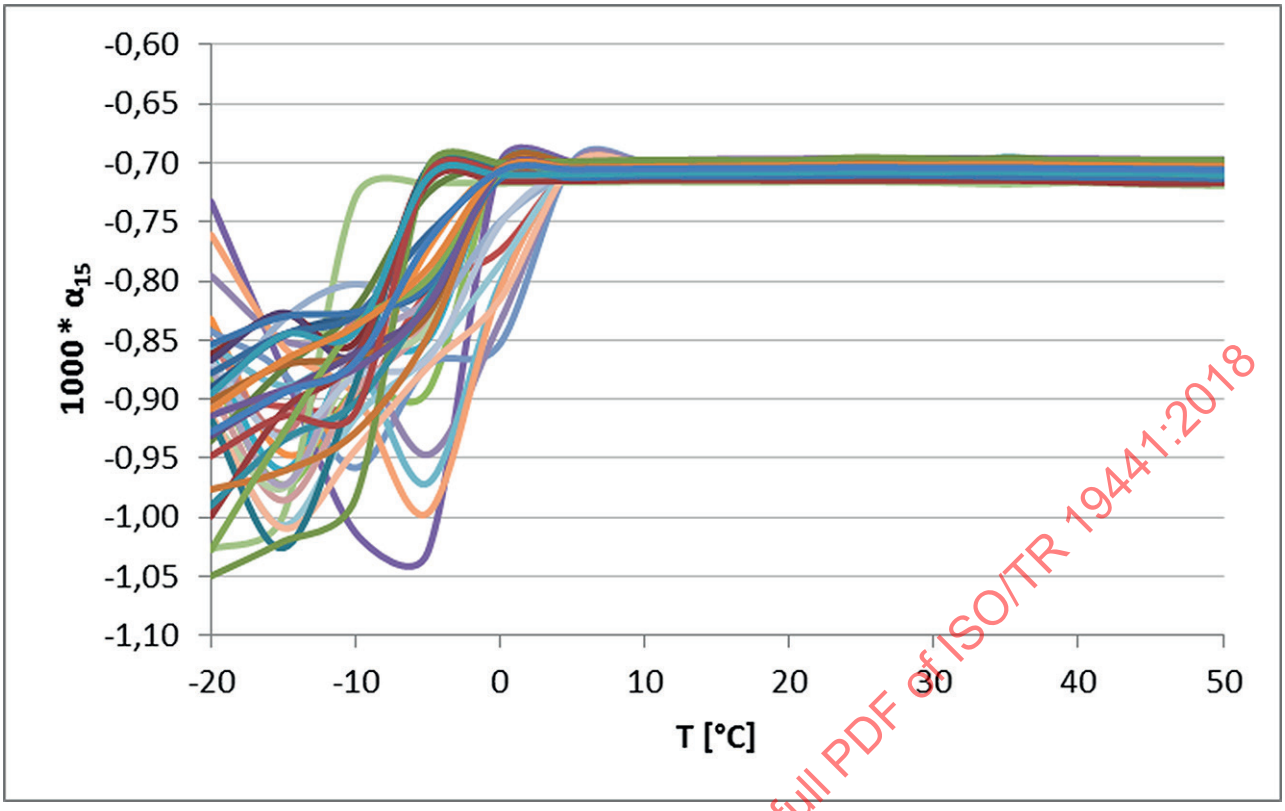


Key

X temperature in °C,

Y [diff of $D(t)1 - D(t)2$] per °C

Figure 6 — Slopes (curvature) of the $D(t)$ function for 18 diesel fuels (winter quality)



Key

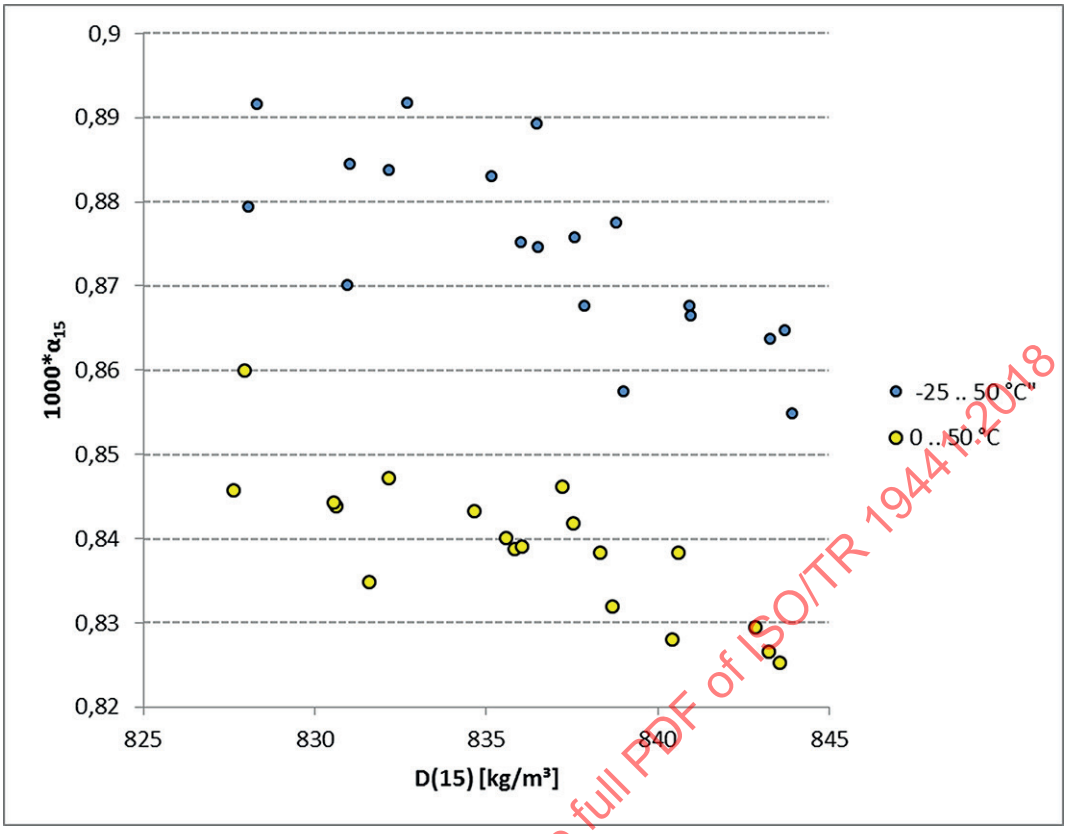
X temperature in °C,

Y [diff of $D(t)1 - D(t)2$] per °C

Figure 7 — Slopes (curvature) of the $D(t)$ function for 20 diesel fuels (summer quality)

This slope behaviour is probably due to solid forming/crystal build-up or similar effects, and because it became clear that it does can have a negative effect on later regression routines, the decision was taken using only a well-behaving temperature range ($t \geq 0$ °C – see the tables).

For the some sample sets, both temperature ranges were used in order to find out how much the reduced temperature range would influence the calculated α_{15} and $D(15)$ values. This information is included in the tabled results as well as in Figures 8 and 9. These figures indicate that the chosen temperature range for calculation of α_{15} and $D(15)$ for a product family can have a very visible effect.

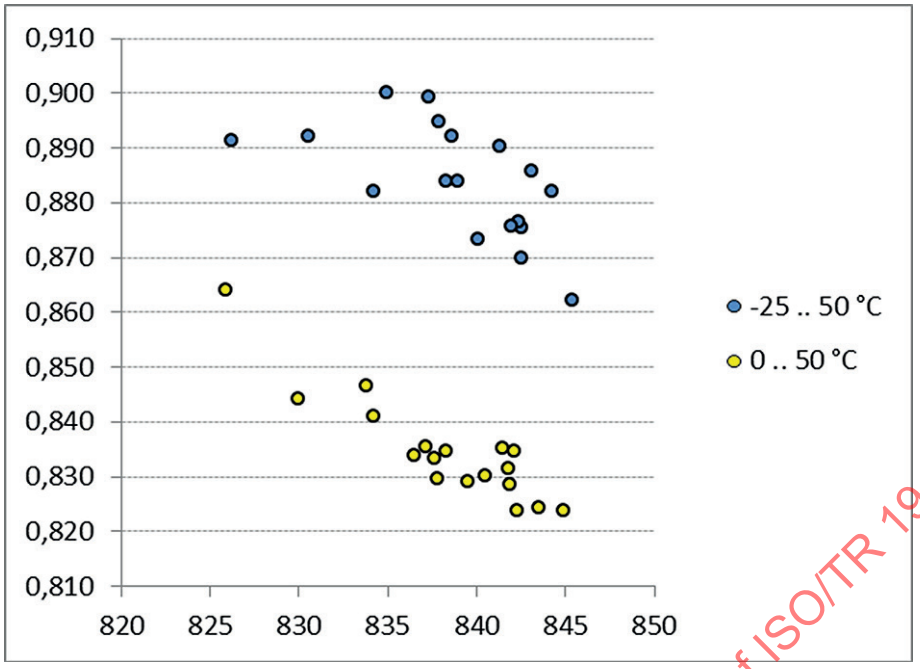


Key

X $D(15)$

Y $1\,000 * \alpha_{15}$

Figure 8 — Temperature ranges calculating α_{15} and $D(15)$ for some DK fuels (winter quality)



Key

X $D(15)$

Y $1\,000 * \alpha_{15}$

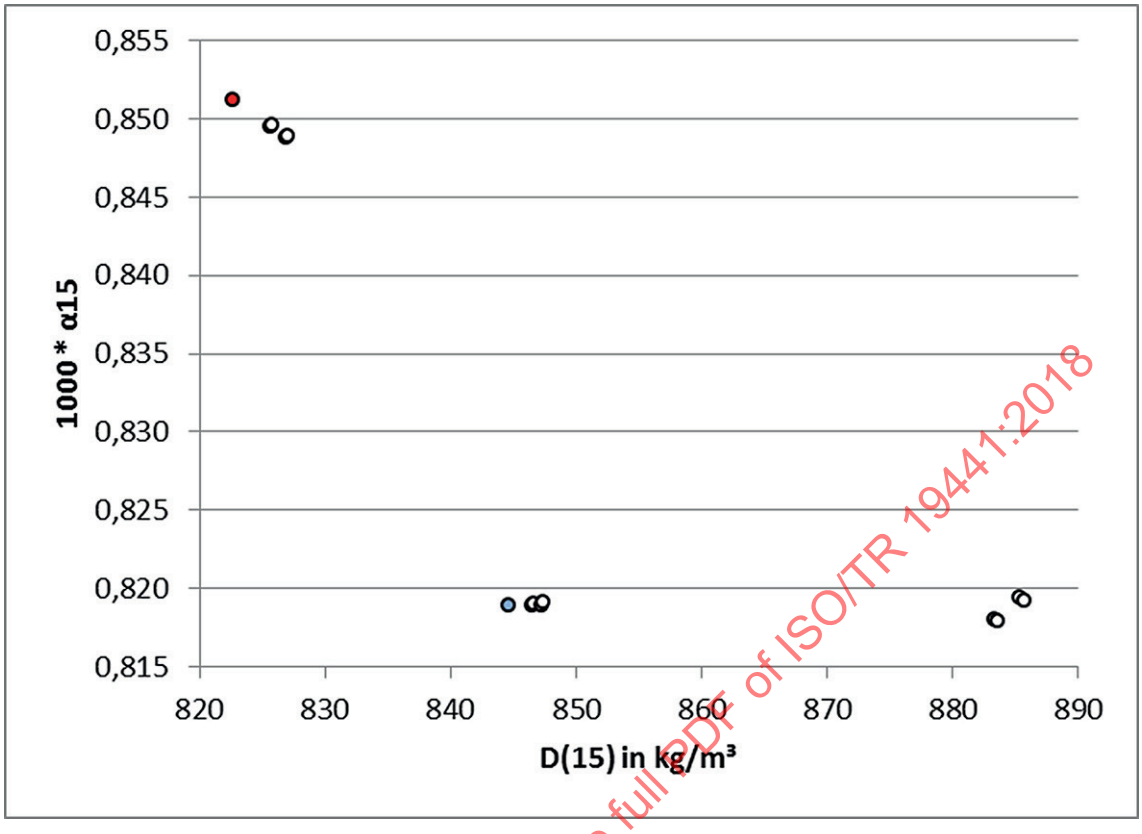
Figure 9 — Temperature ranges calculating α_{15} and $D(15)$ for some DK fuels (summer quality)

11.2.6 Diesel fuels (B0, B5, B7) and more FAMEs

Based on the resulting effect of the selected temperature range, further measurements were executed for a range of 0 °C to 50 °C for some base diesel fuels, base FAMEs, B5 and B5 blends as they can now be found in the EC markets conforming to the corresponding EC fuel specifications (EN 590, EN 14214) (Table D.7).

IMPORTANT — When inspecting the effects of B5 and B7 FAME contents, the CEN fuel specifications currently only specify the maximum FAME content, which means that a B7 fuel can, just like a B5 fuel, contain only about 3,5 %(V/V) FAME or even less.

Figure 10 and the corresponding Table D.7 indicate that variations in the summer/winter base diesel composition have a much larger effect on the resulting [$D(15)$; α_{15}] plot than smaller differences in FAME contents or FAME composition.



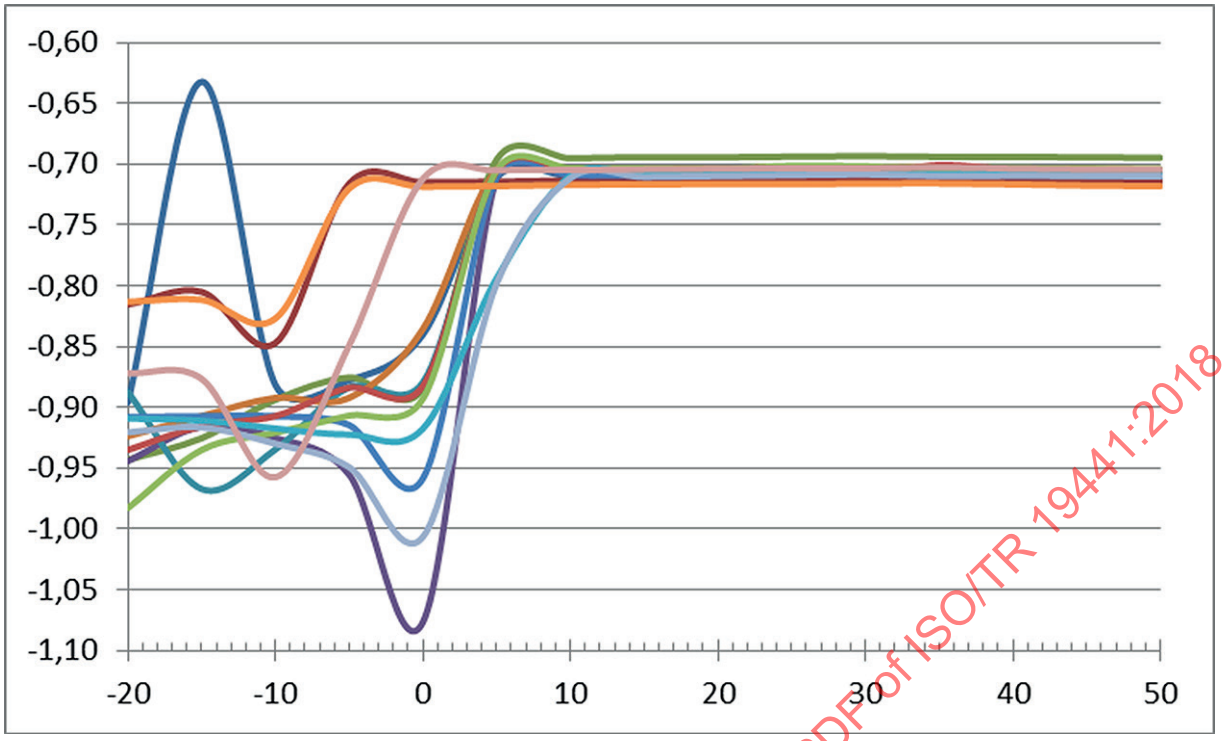
Key

red DK (B0) summer quality
blue DK (B0) winter quality
white B100 and B5, B7 samples

Figure 10 — 1 000 * α15 vs. D(15) for some diesel fuels DK/FAME blends

11.2.7 Domestic heating oils (DIN 51603-1)

A representative set of domestic heating oil samples from summer and winter (according to DIN 51603) was studied (Table D.8), also showing the "abnormal" low temperature behaviour like the other middle distillate samples (see Figure 11). Although $D(t)$ measurements had been executed in a temperature range from −25 °C to 50 °C, only the results for 0 °C .. 50 °C were used to calculate the needed α_{15} and D(15) values.



Key

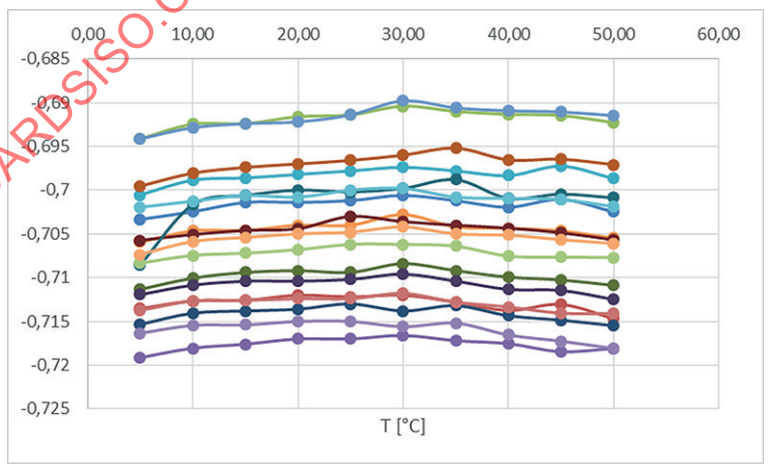
X temperature in °C

Y [diff of $D(t)1 - D(t)2$] per °C

Figure 11 — Slopes (curvature) of the $D(t)$ function for 13 samples of domestic heating oil

11.2.8 Low sulfur domestic heating oils (DIN 51603-1)

A representative sample set of low sulfur domestic heating oils using separate sets of summer and winter grades according to DIN 51503-1 was only examined in the temperature range between 0 °C and 50 °C (see Table D.9 and D.10). In that range no low temperature behaviour was observed.

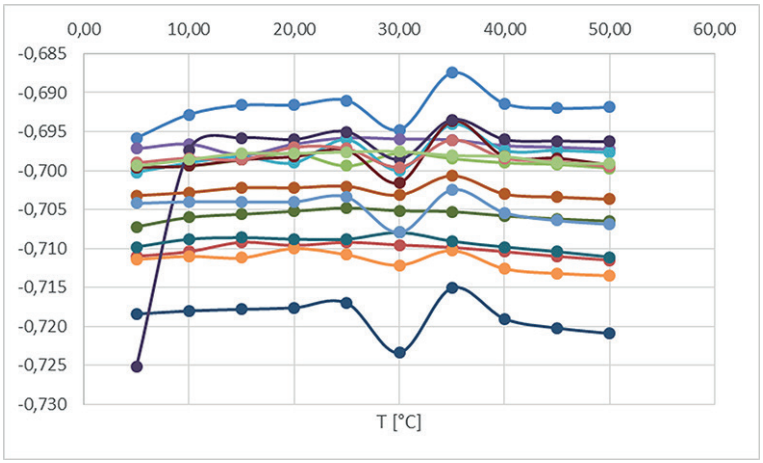


Key

X temperature in °C

Y [diff of $D(t)1 - D(t)2$] per °C

Figure 12 — Slopes (curvature) of the $D(t)$ function for 18 domestic heating oils (winter quality)



Key

X temperature in °C

Y [diff of $D(t)1 - D(t)2$] per °C

Figure 13 — Slopes (curvature) of the $D(t)$ function for 18 domestic heating oils (summer quality)

11.2.9 Rapeseed oil fuels

Table 7 (see also Table D.11) shows some $D(t)$ values for two rapeseed oil fuels according to DIN 51605 which can be used in particular in agricultural equipment with engines adapted to run on such fuels. With just two samples examined, the results for this product family do not claim to be fully representative.

Table 7 — $D(t)$ Values for two rapeseed oil fuels

Temp.	Sample 1	Sample 2
10,0	923,8	924,0
13,0	921,4	921,9
15,0	919,9	920,6
19,0	917,3	917,8
22,0	915,3	915,8
25,0	913,2	913,8
28,0	911,1	911,7
34,0	907,1	907,7
37,0	905,1	905,7
40,0	903,1	903,7
α (60 °F)	0,411 0	0,4067
D (60 °F)	919,70	920,18
α (15 °C)	0,739 9	0,732 1
D (15 °C)	920,08	920,56

NOTE Sample 1: cold-pressed; sample 2: fully refined.

11.2.10 GTL and XTL samples

A set of representative paraffinic diesel fuel samples has been measured by the German metrological office, PTB. These values are shown in Table E.1. The constants proposed for the product family specified in this standard are developed from this table, and a check for the expected maximum calculation error (for a target temperature of 50 °C) is also given in Table E.2.

As a further check, duplicate density measurements for three representative paraffinic diesel fuel (XTL) products (see Table E.3) have been executed which are used here as an additional check to see how well conversion calculations using the constants for "GTL" from Table E.2 do also apply to new XTL samples which have not been included in the modelling. The data in Table E.3 are obtained using K_0, K_1 from Table E.2 (i.e. from the other sample set) according to Formula (E.3) and also including prediction check via calculation of density at 50 °C.

The results show that such extension to other samples of the same product family can be done without problems for a range of densities at 15 °C from about 700 kg/m^3 to 830 kg/m^3 in a temperature range of −20 °C up to 50 °C.

Constants K_0 and K_1 from Table E.2 may be used for samples from this paraffinic diesel fuel product family to execute density/temperature and volume/temperature conversions with sufficient precision following the standardized calculations given in E.2. See Annex E for a detailed discussion of the results.

α_{15} and $D(15)$ data points obtained from this study are not sufficiently close to the published PMT values. This could mean that for this new product family a new set of group constants for the prediction of $D(t)$ values would have to be established.

Annex E was adopted for EN 15940. The constants and formulas to be used for paraffinic diesel fuel products are given in E.4; they were developed based on the calculations given in Annex E.

11.2.11 Summary of results for middle distillate samples

As already explained in previous clauses, the EC Measurement Instrument Directive[16] requests that the maximum difference between predicted and measured $D(t)$ or V(t) values remains at a level of ≤±0,2 % of the measured results. Since potential differences from the prediction model's Lack of Fit increase with the applied temperature differences, we apply a maximum temperature difference of 35 °C here. One can then be sure that the precision requirement will also be met for smaller temperature differences.

The obtained individual data points ($D(t)$; α_{15}, (see Annex D, Table D.12) are plotted in Figure 14, similar to Figure 4, using the already described corridors. Data points inside the boxes show that the published PMT could be used to predict $D(t)$ values for that product. Figure 14 shows the data points obtained for the middle distillate product families FAME and diesel – not all samples are within the EN 590 or EN 14214 specifications.

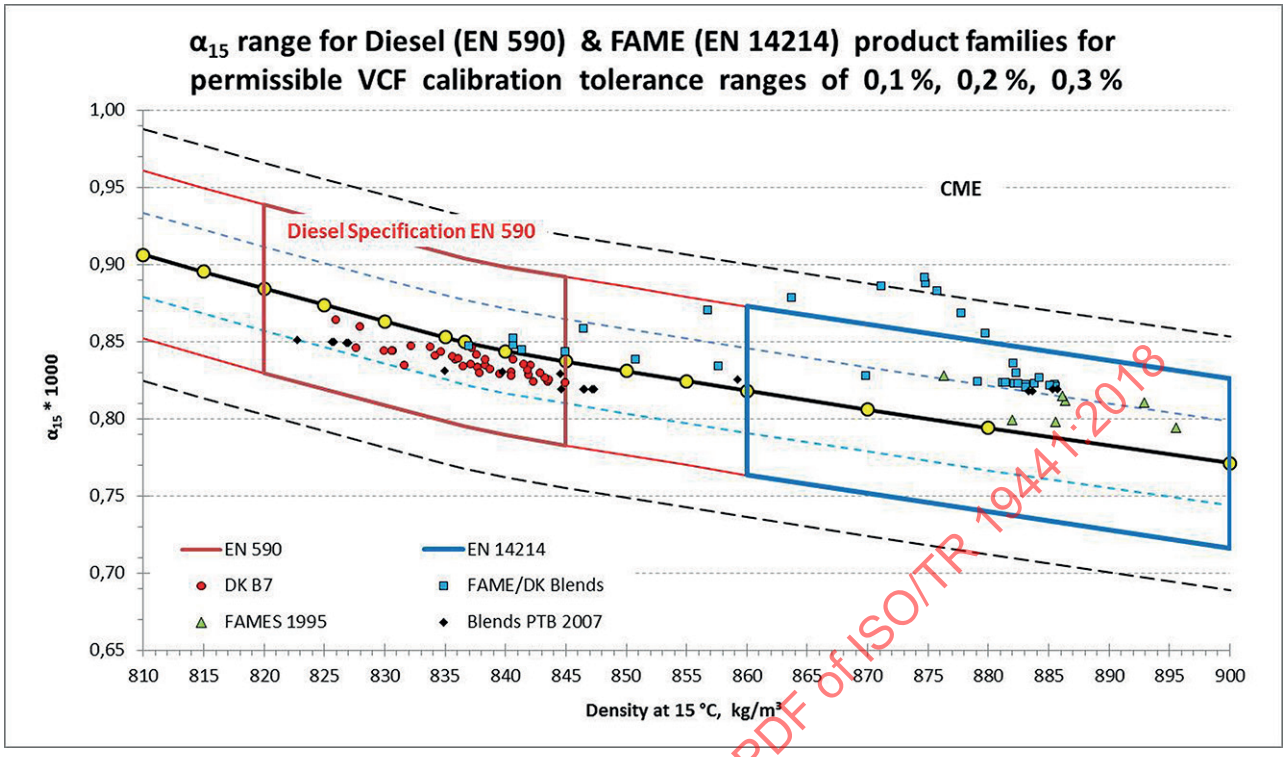


Figure 14 — Fitting obtained MD data into the precision data boxes for diesel fuel and FAME

Figure 14 discloses a number of details.

— All diesel products have an α_{15} which is less than 0,1 % less than values from the published PMT; meaning that although the precision requirements to use PMT are met, there is a small bias.

— FAME samples have an α_{15} which is up to 0,1 % higher than values from the published PMT; so precision requirement for using the PMT are basically met except for samples which contain more than 50 %(V/V) CME.

— The still tolerable small differences to the published PMT values indicate by existence of the visible bias, that Diesel compositions have undergone several changes since the PMT constant have been established.

11.3 Petrol type fuels

11.3.1 EN 228 market petrol fuels

One of the major changes petrol type fuels were facing in recent years was blending ethanol in various shares in order to increase the share of renewable fuels. EN 228 already comprises two different tables for petrols up to 5 %(V/V), E5, and up to 10 %(V/V), E10. Higher blends (E85) are already available, and also other components are under discussion, challenging the validity of the temperature/density functions used for the well-known class of hydrocarbon fuels. Subclause 9.2 covers E0 fuels without ethanol as well as higher blends up to 85 % of ethanol.

Several sample sets were collected and tested in order to cover the different variations of petrol in the European market. In contrast to the observations made for middle distillates, no abnormal low temperature behaviour could be observed so that the full temperature ranges documented could be used. Furthermore, the curvature plots of the $D(t)$ function display clearly a monotonous and nonlinear behaviour (see Figure 17 as just one example) which was also observed for the other examined petrol sample sets. For that reason, alternative linear models or narrowed temperature ranges have not been tested.

11.3.2 Results for EN 228 Super 95 petrol E0 (summer quality)

$D(t)$ results and calculated α_{15} and $D(15)$ values for 17 OK 95 E0 petrol samples are listed in Table D.13. Figure 15 gives a representation of these results.

Further inspection of the results (not displayed here) indicates that the differences between measured and calculated $D(15)$ values are less than about 0,02 of the predicted values (about 10 times less than the precision requirement from the EC Measuring Instruments Directive). It is also worth mentioning that the $D(15)$ span for this Petrol 95 E0 collection is 3,2 %.

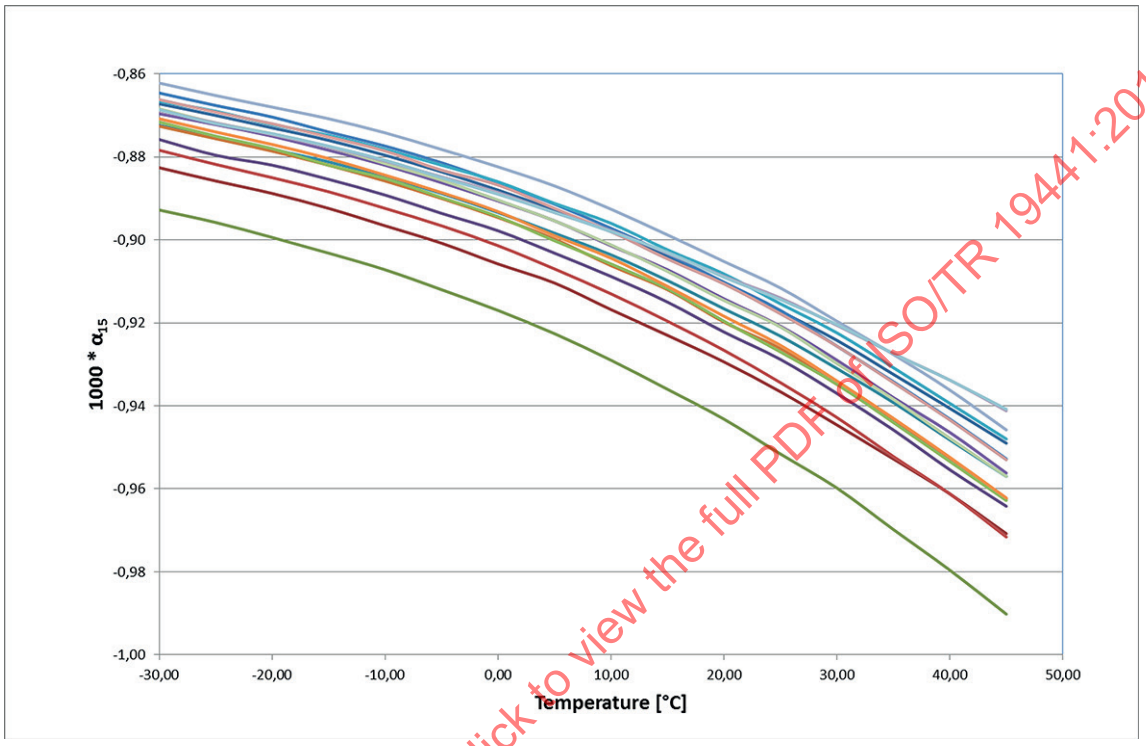


Figure 15 — Nonlinear curvature of the $D(t)$ curve for 17 petrols (E0 –OK 95, summer quality)

11.3.3 EN 228 Super 95 petrols E5 (winter quality)

$D(t)$ results and calculated α_{15} and $D(15)$ values for 16 OK 95 E5 petrol samples are listed in Table D.14. Inspection of these results (see Figure 16) indicates very similar behaviour to Super 95 – E0 given in the previous paragraph. Differences between measured and predicted $D(15)$ is again at the level of 0,02 % of the predicted values (about 10 times less than the precision requirement from the EC Measuring Instruments Directive) and the density span for this E5 sample set id about 4,7 % of the mean D15 value.

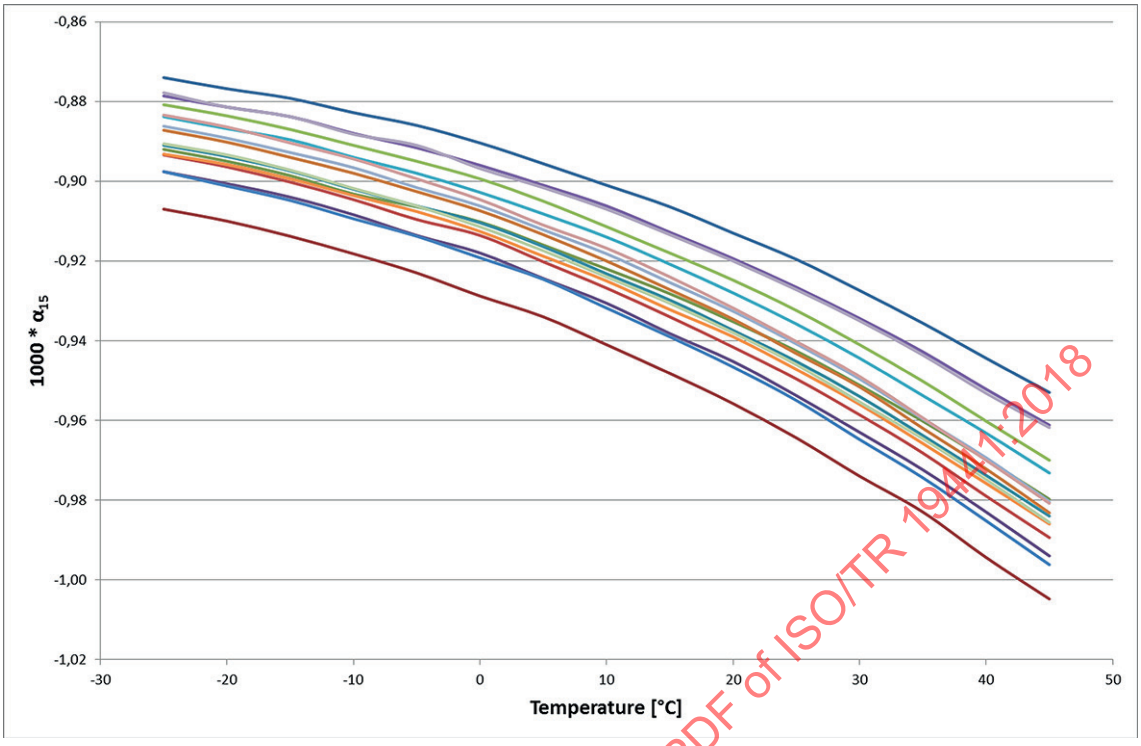


Figure 16 — Nonlinear curvature of the *D*(*t*) curve for 17 petrols (E5 – OK 95, winter quality)

11.3.4 EN 228 Super 95 petrols E10 (winter quality)

Only three samples could be collected and measured due to some shortage of measurement capacity and the recent introduction of E10 to the market at that time. Difference between measured and predicted *D*(15) is again at the level of 0,02 % of the predicted values (about 10 times less than the precision requirement from the EC Measuring Instruments Directive), and the density span for this E10 fuel family has not been calculated. Results are given in Table D.15 and in Figure 17.

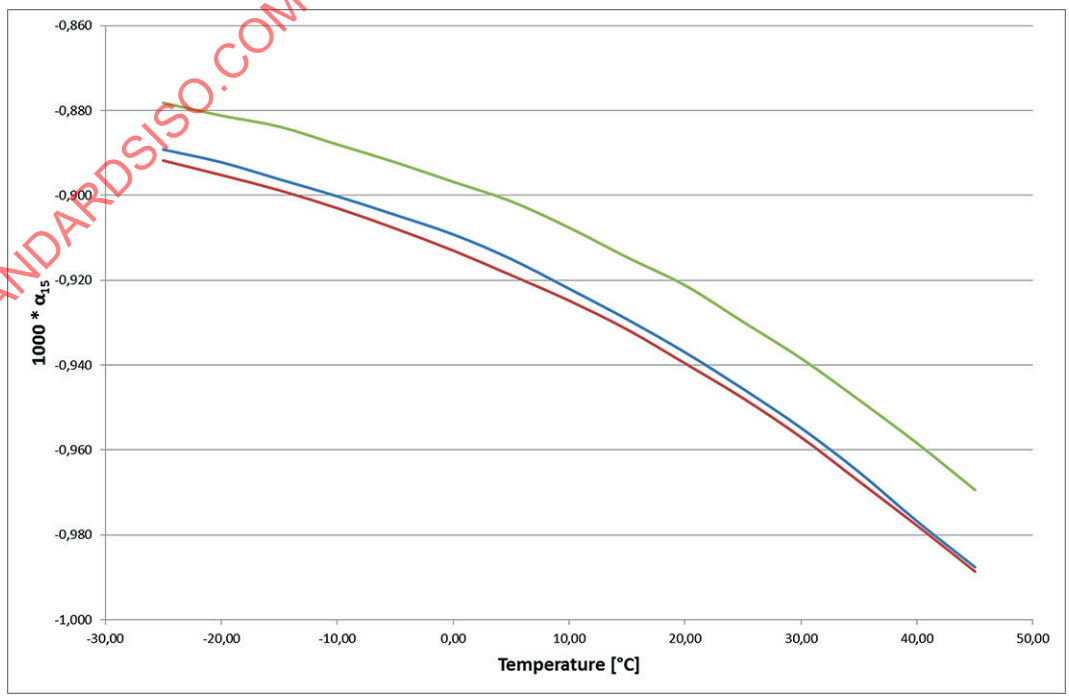


Figure 17 — Nonlinear curvature of the *D*(*t*) curve for 3 petrols (E10 –OK 95, winter quality)

Inspection of these results indicates behaviour very similar to the other reported petrol sample sets. The difference between measured and predicted $D(15)$ stays at the level of about 0,025 % of the predicted value (about 10 times less than the precision requirement from the EC Measuring Instruments Directive).

11.3.5 EN 228 Super 98 petrol E0 (summer quality)

Fourteen Super 98 E0 petrol samples were collected from German filling stations. Inspection of these results (see Table D.16) indicates a similar behaviour to the other petrol samples given in the previous paragraphs. Differences between measured and predicted $D(15)$ is at the level of 0,02 % of the predicted values and the density span for this E5 sample set is about 2,7 % of the mean $D15$ value.

The curvature plot in Figure 18 of the $D(t)$ function contains three samples with different behaviour at the high portion of the temperature range (samples 06, 14, 16). Although no further investigations of this effect have been done, it is assumed that this might have something to do with bubbling or evaporation of some light components, as the effect shows at higher temperatures.

Such effects will not be visible when a linear or other model is used, so especially for unknown or dubious situations the "full treatment" is strongly advocated. This can always be simplified later if need arises.

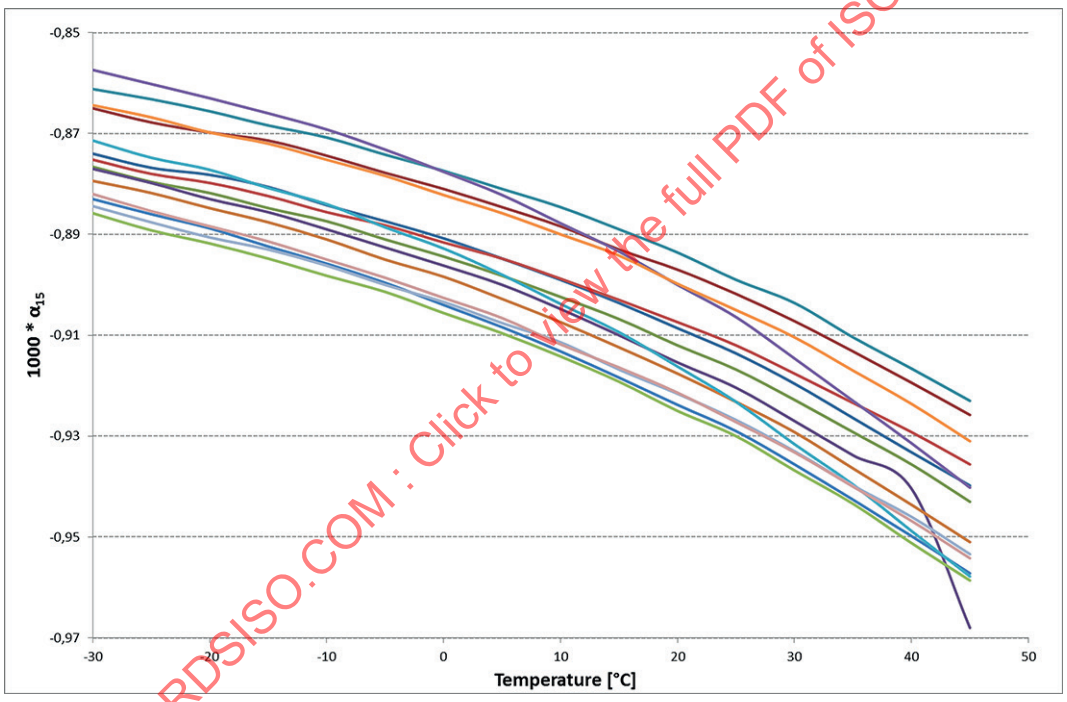


Figure 18 — Curvature of the $D(t)$ function for Super 98 E0 samples

11.3.6 EN 228 Super 98 petrol E0 and E5 (winter quality)

$D(t)$ values and calculated α_{15} and $D(15)$ results for 15 Super 98 petrol samples E0 and E5 are listed in Table D.17. Inspection of these results indicates a similar behaviour to the other petrol samples given in the previous paragraphs (see also Figure 19). Differences between measured and predicted $D(15)$ is at the level of 0,011 % of the predicted values and the density span for this sample set is about 3,8 % of the mean D15 value.

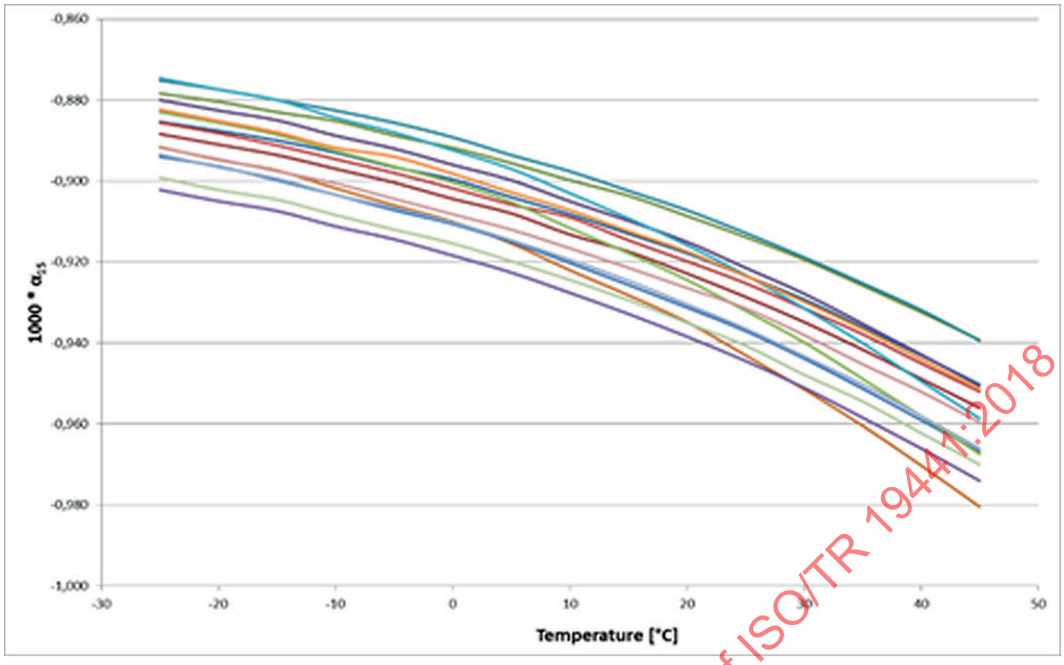


Figure 19 — Curvature of the $D(t)$ function for Super 98 E5 and E0 samples

11.3.7 EN 228 Super 98 petrols E0 blends with different shares of ethanol

In order to get a better picture of the full range (E0 to E100) petrol behaviour, a number of blends have been prepared and examined [see Table D.18 for $D(t)$ values and calculated $\alpha 15$ and $D(15)$ results]. Several similar investigations, e.g. at the API, have been mentioned, but even on repeated request details from that program had not been made available for this document.

Inspection of these results indicates a similar behaviour to the other petrol samples given in the previous paragraphs. Differences between measured and predicted $D(15)$ is at the level of 0,02 % of the predicted values and the density span for this sample set is about 7,9 % of the mean D15 value.

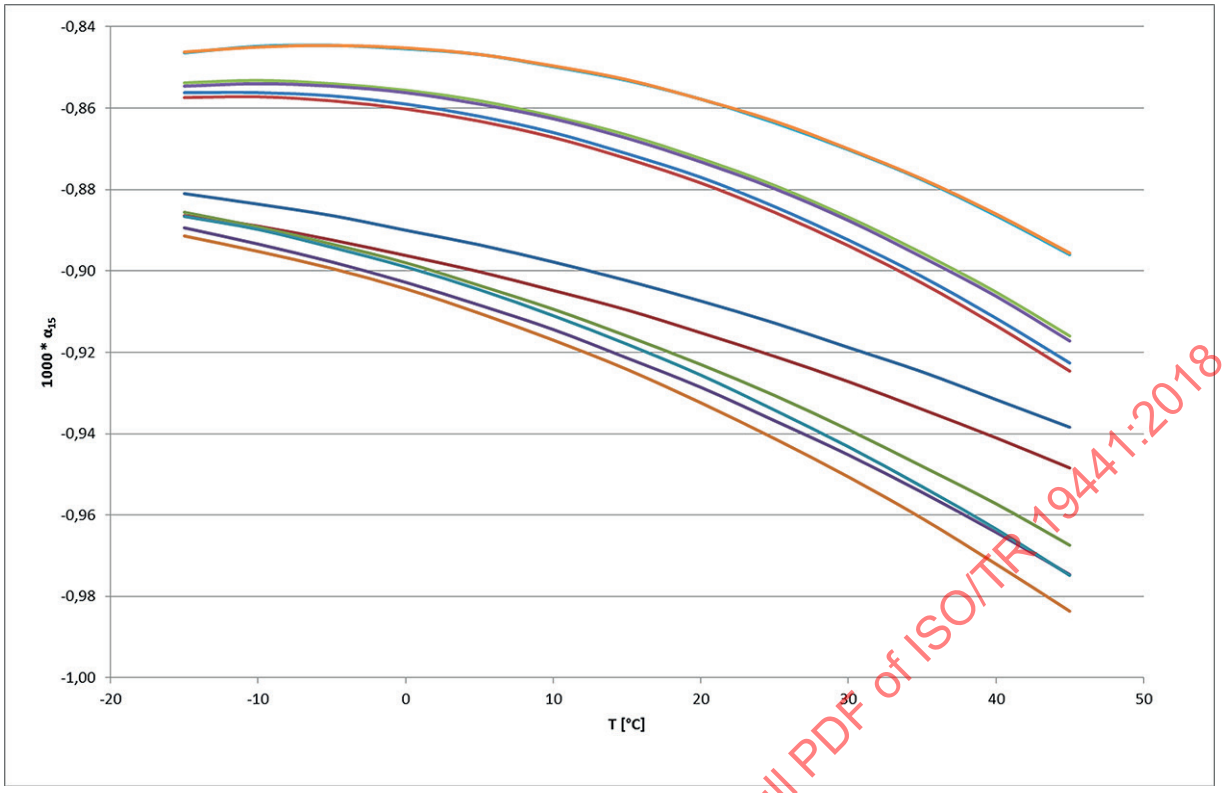
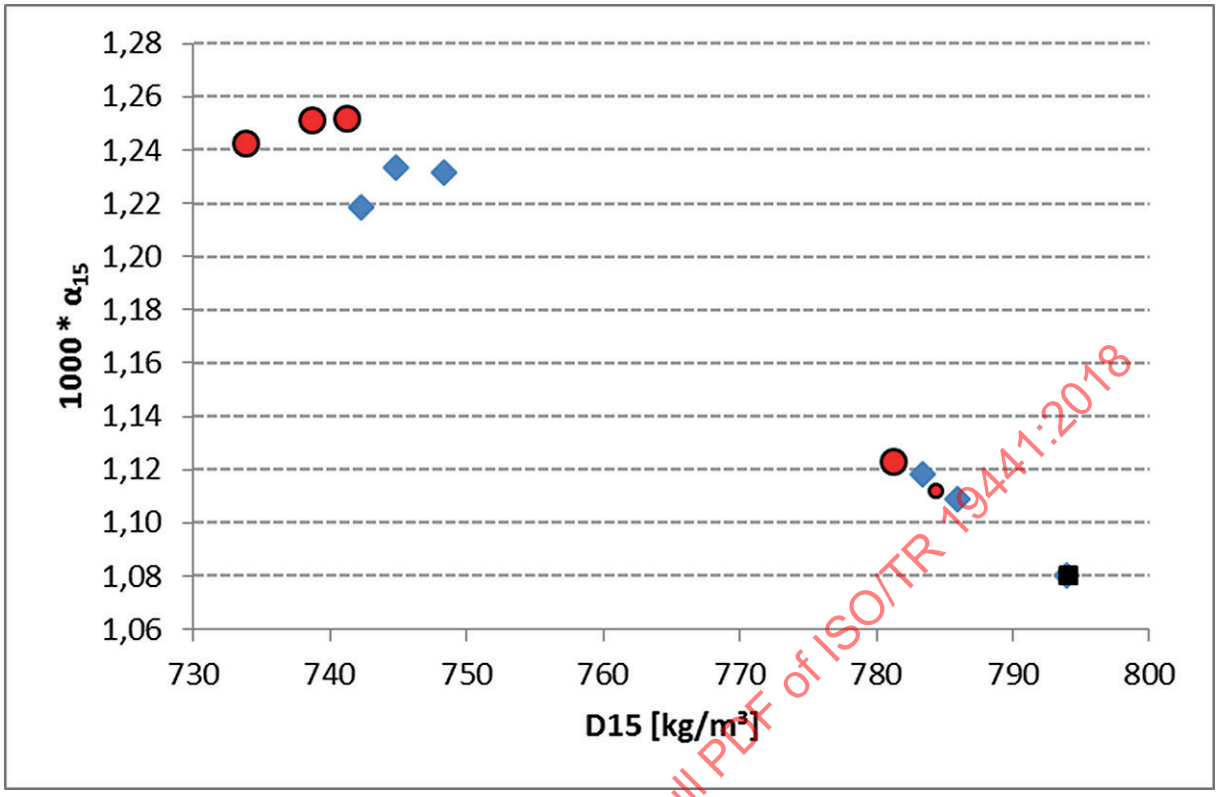


Figure 20 — Curvature of the *D*(*t*) function for a set of petrol blends (E0 .. E100)

Figure 20 indicates very clearly the differing and monotonous curvatures of the members of this sample set.



Key

red winter quality
blue summer quality
black E100 (ethanol)

Figure 21 — α_{15}; $D(15)$ plot for the sample set of blends (E0 .. E100)

Figure 21 gives some important additional information.

— The position of a sample on this plot is mainly controlled by the composition of the fuel part, which can be quite different as the data points for summer and winter indicate.

— The position for ethanol (with only little compositional variation) does not change much.

— As opposed to a normal linear blending behaviour, an interesting nonlinear effect is seen for samples with up to 10 % ethanol.

Similar effects had been found in the first blending exercises for E5, where an excess vapour pressure had been detected. Here, one would assume a similar effect of the molecular solution effects ("Lösemittelkäfig") for the mixture of non-polar and very polar constituents. As the ethanol content increases, this effect is diminished.

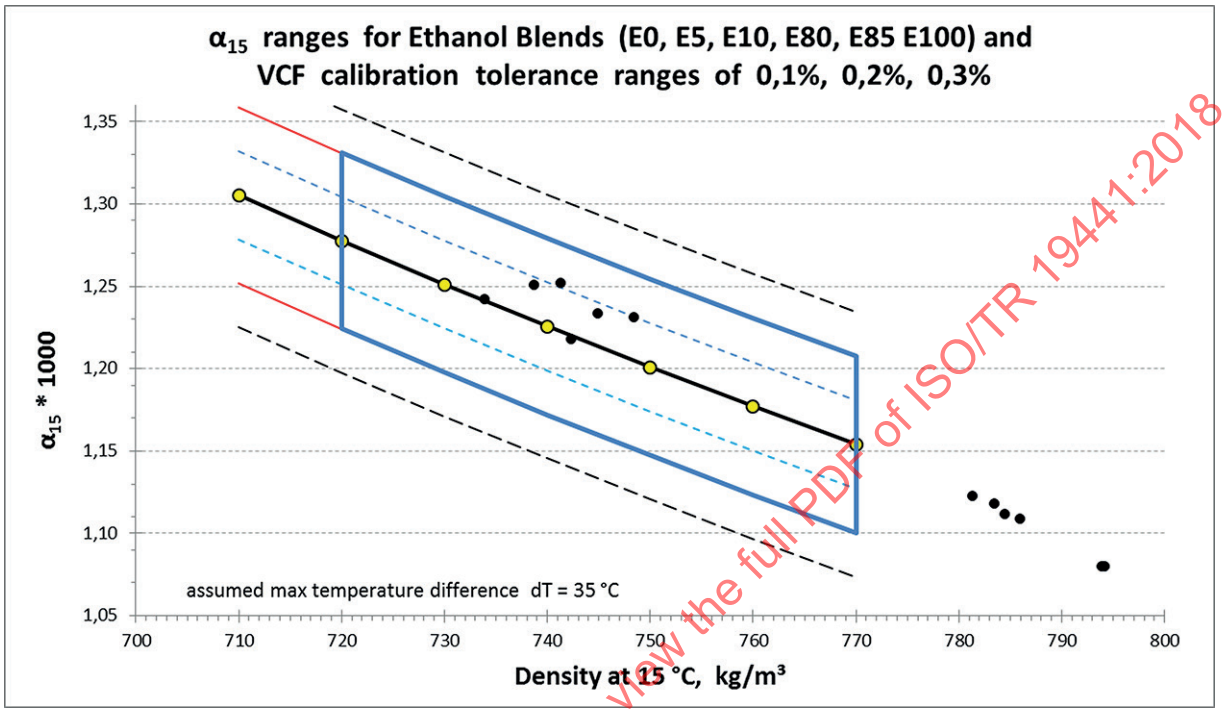
11.3.8 Conclusions for $D(t)$ behaviour of the petrol fuel samples

Figure 22 displays the calculation results for the E0 to E100 blends discussed in this section (see also Annex D, Table D.19). While the currently specified EN 228 fuels fall well into the allowed region, this is not the case for the E100 and E85 samples, meaning that starting from and above about 40 % to 50 % ethanol content, the published PMT tables cannot be used any longer.

NOTE 1 A clear cut between the allowed and disallowed regions cannot be made based on the obtained data because this dividing line depends to the most part on the base fuel composition as already the differences between the summer and winter qualities indicate.

NOTE 2 The main reason for the forbidden use of the published PMT data is ruled by the fact that at the upper $D(15)$ limit of the EN228 petrol specification the PMT requires a switch to another set of group constants (K_0, K_1, K_2) for Naphtha.

NOTE 3 Abandoning this PMT requirement to switch to the naphtha group constants and keeping the group constants for Petrol (K_0 = 346,4228; K_1 = 0,4338, K_2 = 0) also for the $D(15)$ range above the EN 228 specification could allow rather well functioning VCF/α_{15}, $D(15)$ model calculations even for E85 type fuels. However, so far no discussion about any such change in the PMT rules has been held.



Key

black line + yellow dots	data from the published PMT tables
black dots	Exx samples
broken lines	tolerance ranges of 0,1 %, 0,2 % and 0,3 %
blue box	density limits and 0,2 % tolerance range for EN 228 (for further explanations, see text below)

Figure 22 — Plot of E0 to E100 blends in $D(15)$; α_{15} data space

Annex A
(informative)

Calculation of alpha60F, D60F and alpha15 plus D15 for a set of single unknown petroleum samples according to API MPMS Chapter 11.1

A.1 Background

The script presented here has been used over the years to check published values as well as to obtain reliable $\alpha 15$ and $D15$ data for samples from new product families mostly of biological origin. The obtained values have then been used for comparison with values from the published PMT tables in order to find out if the old values would still be appropriate or if some new constants had to be developed for some new product families.

In order to obtain valid α_{15} values for a whole new product family, a sufficient number (a minimum of 10; more samples are better) of representative family members which cover the most probable compositions has to be examined, covering the density and temperature ranges of interest. For each sample, minimum 10 density/temperature pairs are determined at that temperature range. Due to some regulatory issues and some practical ones as well, the most often temperature range for liquid fuels is normally from about –20 °C to 50 °C. It is, however, important to note that irregular sample behaviour (like solidification, crystal formation, bubbles and boiling) should be avoided. If has also been shown during the course of this project that the chosen temperature limits do have some influence on the calculated thermal expansion coefficient, "α" and density, although we have not explicitly presented that type of side result.

The calculations centre around a nonlinear regression according to the exponential model as described in the main text. The whole object then is to get, for each investigated sample a sample specific thermal expansion coefficient α_{15}, which are reported together with the reference density D(15 °C). In addition we report also the calculated results for "α_{60F}" and the density at 60 °F.

NOTE All encountered "α_{15}" values fall into the range from about 0,6*10^{-4} to 1,5 * 10^{-4}. For easier writing and reading e.g. in the attached tables, we report the value 1 000 *"α15". This, of course, needs to be remembered when the printed values are used in the exponential model.

After such individual constants have been calculated it is highly recommended to check how well they can be used for the prediction of densities at higher (and also lower) temperatures. The differences between measured and predicted values e.g. for a rather large temperature difference of (50–15) °C should smaller than the required regulatory max prediction error (0,2 %) in Europe, so e.g. $D_{50°C,predicted}/D_{50°C,measured}$ should not be larger than 1,002 or less than 0,998. If this condition is met for the "extreme temperature" of 50 °C, it will also hold for temperatures less far away from the reference 15 °C.

A.2 The statistical software

The statistical software "R" is a very robust, comfortable, reliable object oriented scripting language from the public domain which is not only used in industry but also for large research projects in many universities, so it can be assumed that most enclosed calculation routines are as reliable and error free as at all possible. However, a scripting language also has the danger that uncontrolled changes are made willingly or unwillingly to the script, which means that some care should be exercised when this software is applied. The software can be downloaded for free (see Reference [36]).

The script α_{15} and $D(15)$ presented later in this clause follows closely the basic routines presented in DIN 51757, API MPMS Chapter 11.1 and many other scientific papers. These are exactly the same routines which have also been used for many years for the development of constants for the conventional products which have been in the market for decades. The script assumes the presence/input of min. 10 paired values of temperature in °C and density at that temperature (normally in kg/m^3), but the script does not check for this. Also, the results α_{60F}, $D(60\ °F)$, α_{15} and $D(15\ °C)$ are calculated separately for each sample, but the format of the input data file allows simultaneous input of data for many samples as a batch, when the sequence of used temperatures are the same for all samples. If that is not the case, samples with different temperature profiles should be input as separate files.

WARNING — We have deliberately not produced a compiled program so that any user who wants to use this program can find out exactly how the calculations work. Use it at your own risk or better even leave the work to the experts – you will not need to use this in daily routine. And another word of caution: this scripting language is case sensitive, so better be careful when you want to edit the source text.

A.3 Installation of the *R* software package

For installation, just download the packages and install them. There are hardly any unusual obstacles. In addition to the original *R* packages, we recommend to use also a very convenient IDE from the public Domain called R_{Studio}. After installation is complete, copy the R-script below plus any input data files into just one convenient directory. Then start R_{Studio}, open the script file and set the working directory to the directory of the script file.

Press ctrl-A to select all lines of the script and then ctrl-R to run it. The results will be saved to the same directory (which can even sit on an memory stick).

The structure of our input data file has is a simple Excel CSV format, which makes it quite easy to track potential errors with a text editor and which allows further processing with all kinds of other software. The content in cell A1 is temp which is used to identify this data format.

This is the data format (self-explanatory) except maybe for the decimal comma used in Germany.

((Input File))			((Output File))	
temp	samp1	samp2 … … …		
14,9	868,21	768,21		
15,9	867,50	767,50	samp1	alpha60F = 0,446 66
20,2	864,51	764,51		D60F = 867,756
25,0	861,19	761,19		alpha15C = 0,803 98
29,6	857,91	757,91		D15C = 868,144
32,9	855,62	755,62		
35,4	853,82	753,82	samp2	alpha60F = 0,504 44
40,2	850,48	750,48		D60F = 767,754
42,0	849,16	749,16		alpha15C = 0,907 99
44,9	847,15	747,15		D15C = 768,142

The output file has a similar name (with -res added to it to separate it from the input file. It is also an Excel CSV file listing sample name, alpha60F, D60F, alpha15 and D15 as one line per sample.

Anybody can use that script for free and at his own risk, but when changes are made, please take the pain and rename the source code and the program file name, to avoid later confusion.

```
s##=============================================================================
## R script “alpha-calc,R” Rev, 6,5 - last check in November 2015
## developed by Dr, H,T, Feuerhelm at DIN-FAM, Hamburg, Germany
##=============================================================================
## for calculation of alpha60F, D60F, alpha15C, D15C for new product and
## bio-product samples on the basis of API MPMS Chapter 11,1
## ------------------------------------
## Users of the program should be aware that they use it at their own risk
##=============================================================================

## set no of decimal places you want to use in calculations ,,
## ------------------------------------
options(digits=16) ## change to up to 22 places
##        ## but nor need to do this precision-wise ...,
## change NAME of INPUT and OUTPUT Files here (without file extension)
## ------------------------------------
ifnam<- “DT12-FAMES-Parr”; ifname<- paste(ifnam,”,csv”,sep=””)
ofnam<- ifnam; ofname<- paste(ofnam,”-res”,”,csv”,sep=””)
## Now define some convenient functions
# -- make a first construction data set “densref” for output of results
## ------------------------------------

TestSample<- c(0,446661, 867,756, 0,803082, 868,144) ## just some numbers
resdat<- data,frame(TestSample,
row,names=c(“ Alpha(60F)”,” Density(60F)”,
“ Alpha(15C)”,” Density(15C)”))
densref<- t(resdat) ## -- transpose for better looks
## Conversions for Celsius and Fahrenheit scales
c2f<- function(x) { ergebnis<- 1,8*x+32 ; c2f<- ergebnis }
f2c<- function(x) { ergebnis<- (x-32)/1,8 ; f2c<- ergebnis}

## conversion of temperature scale from ITS90 back to IPTS68
## as required in MPMS chapter 11,1,5,3
## ------------------------------------
ipts90_68<- function(s_rein, x, s_raus) {
a1<- −0,148759; a2<- −0,267408; a3<- 1,080760; a4<- 1,269056
a5<- −4,089591; a6<- −1,871251; a7<- 7,438081; a8<- −3,536296
if (s_rein==“F”) { t<- (x-32)/1,8 }
if (s_rein==“C”) { t<- x }

tau<- t/630
DELT<- (a1+ (a2+ (a3+ (a4+ (a5+ (a6+ (a7+ a8*tau)
*tau)*tau)*tau)*tau)*tau)*tau)*tau
if (s_raus==“C”) { t68<- t - DELT }
if (s_raus==“F”) { t68<- (t-DELT)*1,8 + 32 }
ipts90_68<- t68 }
## begin of iteration function
## ------------------------------------
iterate_a<- function(n,SP,SPP,ST,STP,STT,STTP,STTT,STTTT) {

delt60<- 0,01374979647
a0<- STP - SP * ST/N
a1<- STT + 1,6*(STTP+delt60*STP) - (ST^2 + 1,6*(STT+delt60*ST)*SP)/N
a2<- 2,4 * (STTT + delt60*STT - ST*(STT+delt60*ST)/N)
a3<- 1,28* (STTTT+ (2*STTT+ delt60*STT)*delt60
- (STT+delt60*ST)^2/N)
alpha_start<- a0/(ST^2/N - STT)
```

```
## begin the loop (7 loops are sufficient - could be set higher ,,)
## ----------------------------------
for (I in 1:7) {
dalpha<- -(a0 +(a1 +(a2+a3*alpha_start)*alpha_start)*alpha_start) /
(a1 + (2*a2 + 3*a3 * alpha_start)*alpha_start)
alph0<- alpha_start + dalpha
alpha_start<- alph0
}
## End of loop=====

iterate_a<- alph0
}
## End of iterate function and End of Function definitions
##----------------------------------
## Now read csv input file (n samples, m temperatures) into data-frame
## "daten" - see example given in the text above
## PLEASE NOTE: the German Data format used here requests a DECIMAL comma,
## therefore the function "read,csv2" is used, Now when the csv data file
## uses a decimal point, simply change that function to "read,csv" ,,,,
daten<- read,csv2(ifname,header=T)
## find no of samples in data file andlist of teperatures (Celsius)
## ----------------------------------
anz_proben<- length(daten)
tmc<- daten$temp

##=================================================================
## Start main loop over all samples
##=================================================================
for (j in 2:anz_proben)
{
dm<- daten[,j]
##================create some more variables=======================
tmf<- c2f(tmc)  ### Celsius to Fahrenheit
tstar<- ipts90_68("F",tmf,"F") ### convert to 1968 temperature scale
delti<- tstar - 60,00687490      ### temp-diff in F
lnDi<- log(dm)  ### ln for density
N < - length(tmc)
Sp<- sum(lnDi); Spp<- sum (lnDi^2)
St<- sum(delti); Stp<- sum(delti*lnDi)
Stt<- sum(delti^2); Sttp<- sum(delti^2*lnDi)

Sttt<- sum(delti^3); Stttt<- sum(delti^4)
## now calculate alpha(60F)----------------------
alpha60<- iterate_a(N,Sp,Spp,St,Stp,Stt,Sttp,Sttt,Stttt)
## convert alpha(60F) to alpha(15,66667C),,,,
alpha15c<- alpha60*1,8
## Calculate D(60F)==D(15,66667C)
## and convert to D(15C) - easy: just calculate new D(59F)
## ----------------------------------

ds_help<- Stt+0,01374979647*St
dens60<- exp((Sp +(St + 0,8 *ds_help*alpha60)*alpha60)/N)

dens15c<- dens60*exp(-alpha60*(–1)*(1+0,8*alpha60*(–1)))
## Collect data and results into one variable for output
## ----------------------------------

yy<- c(rounD(alpha60*1000,5), rounD(dens60,3),
rounD(alpha15c*1000,5),rounD(dens15c,3))
densref<- rbinD(densref,yy)
```

```
## now copy sample name from input file and "all done" ,,,
## ----------------------------------
row,names(densref)[j]<- colnames(daten)[j]

} ## END of main loop
densref ## show once on screen for reference

## now save results from "densref" to an output file (CSV)
## ----------------------------------

write,csv2(densref,file=ofname) ### Finito la musica ,,
##----------------------------------
```

The calculated results DT-12-FAME-PARR-res.csv are given in Table A.1. Please note that the calculated (predicted) $D(15)$ results differ a little from the input $D(15\ °C)$ values. This is explained by the two different types of error: while the measured value compares to repeatability and reproducibility of the test method EN 12185, the predicted value only inherits the lack of uncertainty from the regression.

Table A.1 — Calculation results for 12 FAME samples

	α(60F)	D(60F)	α(15C)	D(15C)
PR,1	0,450 89	881,715	0,811 61	882,113
PR,2	0,450 93	882,021	0,811 67	882,419
PR,3	0,451 31	880,772	0,812 35	881,169
PR,4	0,451 77	880,986	0,813 18	881,384
PR,5	0,451 11	885,054	0,811 99	885,453
PR,6	0,450 52	883,324	0,810 93	883,722
PR,7	0,489 46	874,168	0,881 02	874,596
PR,8	0,454 26	881,807	0,817 67	882,208
PR,9	0,450 72	882,573	0,811 3	882,971
PR,10	0,450 43	882,67	0,810 78	883,068
PR,11	0,465 34	840,225	0,837 6	840,616
PR,12	0,463 75	844,523	0,834 75	844,915

The evaluation described here will deliver a set of paired $D15$ and α_{15} values for individual samples. In order to find group constants for a whole product family, another regression can be made if there is sufficient confidence in the completeness and representability of the available data. This approach is not new as it has been used especially for Group B products in the PMT for many decades.

The regression is of the form $\alpha_{15} = K_0/D_{15}/D_{15} + K_1/D_{15} + K_2$.

The resulting triplets K_0, K_1, K_2 then represent the group constants for that product family. This procedure has been used worldwide for many decades. More explanations and detail as well as some history is given in Clause 6 of this document.

Annex B
(informative)

Examples of Y table results in German DIN 51757

DIN 51757[17] describes measurement compatible to ASTM D1250 or IP 200 and makes use of:

— ISO 3675 – Hydrometer Method;

— ISO 3838 – Pyknometer Method[32];

— ISO 12185 – U-Tube Oscillator Method.

DIN 51757 has a so-called Y model for the determination of α_{15}. It is quite similar to the exponential model with the exception that K in the exponent becomes to be a second regression parameter instead of keeping it at a constant value of K = 0,8. The procedure for this two parameter regression is described in DIN 51757 so it does not need to be repeated here. Please note that both α_{15} and K are now regression constants

$$VCF = \exp\left(-\alpha_{15} * (t-15) * \left(1 + K * \alpha_{15} * (t-15)\right)\right) \quad \text{(B.1)}$$

The so-called Y-table finds its main use for pure petrochemical products, where compositional changes are very small and where more precision for the predictions is wanted. Table B.1 shows some data from this Y-table in DIN 51757.

Table B.1 — Data from DIN 51757 Y table for some petrochemicals and oxygenates

Product	$\alpha_{15} * 1\,000$ (in 1/°C)	**Constant** K	D(15 °C) (in kg/m³)	**Valid temperature range** (°C)
Propane	2,850	1,55	507,6	−10 .. 40
Propene	3,095	1,36	523,1	−10 .. 40
Butane	1,900	0,80	584,5	−10 .. 40
Isobutane	2,130	1,00	563,0	−10 .. 40
Isobutene	2,060	1,45	600,1	−10 .. 40
cis-2-Butene	1,900	0,80	627,0	−10 .. 40
trans-2-Butene	1,910	1,33	610,1	−10 .. 40
1-Butene	1,955	1,30	602,1	−10 .. 40
1,3-Butadiene	1,972	0,80	627,7	−10 .. 40
Methanol	1,155	−0,38	796,1	0 .. 40
Ethanol	1,078	0,86	793,5	−20 .. 40
Isopropanol	1,027	0,93	789,1	0 .. 30
Isobutanol	0,923	0,82	805,6	0 .. 30
MTBE	1,413	0,95	745,6	0 .. 30
TAME	1,204	1,72	775,0	15 .. 30
Benzene	1,188	0,68	884,2	0 .. 30
Toluene	1,060	0,73	871,6	0 .. 30
o-Xylene	0,954	0,78	884,3	0 .. 40
m-Xylene	0,983	1,03	868,4	0 .. 30
p-Xylene	0,990	1,30	865,3	15 .. 40

Annex C
(informative)

Precision results for FAME from a German precision determination exercise

C.1 Basics

The results of this precision study at four different temperatures has been executed in 2007 using ISO 4259 procedures with volunteering expert laboratories from the German standardization committee.

— Precision study for 10 FAME samples at 10 °C

— Precision Study for 10 FAME samples at 15 °C

— Precision Study for 10 FAME samples at 25 °C

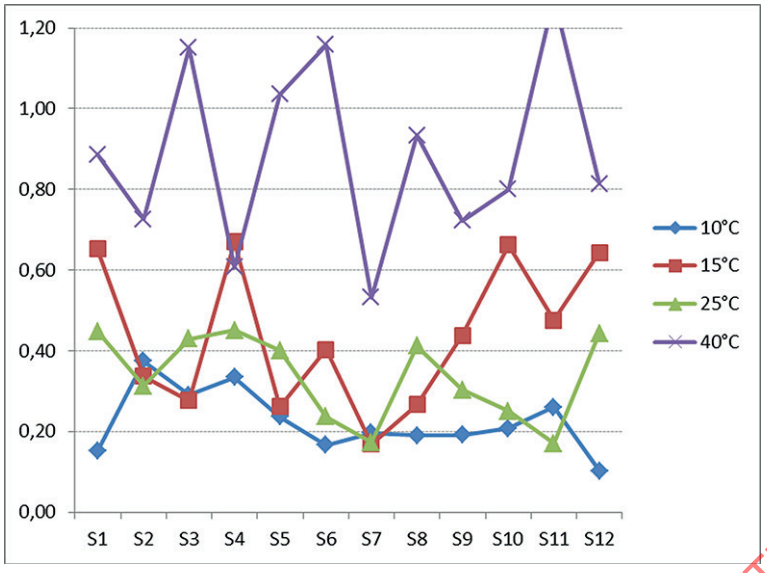
— Precision study for 10 FAME samples at 40 °C

The sample compositions for these 12 samples were as follows:

S1	B100 (RME)	S7	B100(CME)
S2	B100 (RME)	S8	B100 (RME+CME = 90 + 10)
S3	B100 (RME)	S8	B100 (RME+CME = 99,25 + 0,75)
S4	B100 (RME+PME = 90+10)	S10	B100 (RME+CME = 99,995 + 0,005)
S5	B100 (SME	S11	B20 (Diesel B5 + RME)
S6	B100 (RME+SME = 75+25)	S12	B30 (Diesel B5 + RME)

C.2 Discussion

The results suggest differing precision values when measurements are done at elevated temperatures (e.g. 40 °C) which have been judged important. After repeated discussions and inspection of local measurement conditions it was concluded that in some laboratories, the waiting time to arrive at a stable set temperature level had not always been in control. Figure C.1 shows the differences for *R* found for different temperatures.



Key

X sample ID

Y reproducibility

Figure C.1 — Reproducibility *R* found for 12 FAME samples at four different temperatures

It seems worth mentioning that the test method's precision statements do not cover such temperature effects, nor does the standard contain any clear indication which of the two precision statements should be applied exactly to which product type.

Table C.1 — $D(t)$ Measurements for 10 FAMES and 2 diesel fuels at 31 temperatures (all >> 0 °C)

temp (°C)	PR.1	PR.2	PR.3	PR.4	PR.5	PR.6	PR.7	PR.8	PR.9	PR.10	PR.11	PR.12
70,00	842,357	842,655	841,422	841,587	845,535	843,937	831,756	842,157	843,201	843,320	801,471	805,708
68,00	843,813	844,098	842,872	843,035	846,989	845,384	833,319	843,610	844,648	844,766	802,902	807,144
66,00	845,260	845,546	844,322	844,487	848,442	846,834	834,885	845,071	846,096	846,214	804,337	808,577
64,00	846,709	846,995	845,767	845,938	849,894	848,283	836,449	846,530	847,544	847,660	805,767	810,011
62,00	848,156	848,445	847,215	847,387	851,349	849,728	838,013	847,988	848,993	849,108	807,199	811,442
60,00	849,603	849,894	848,661	848,835	852,803	851,178	839,580	849,447	850,440	850,556	808,629	812,874
58,00	851,046	851,339	850,110	850,284	854,256	852,624	841,140	850,906	851,888	852,000	810,057	814,305
56,00	852,494	852,786	851,555	851,733	855,708	854,073	842,701	852,362	853,335	853,447	811,485	815,735
54,00	853,941	854,235	853,001	853,183	857,161	855,522	844,262	853,820	854,781	854,892	812,912	817,163
52,00	855,386	855,679	854,447	854,629	858,612	856,968	845,824	855,279	856,229	856,338	814,338	818,591
50,00	856,831	857,128	855,893	856,075	860,066	858,415	847,381	856,734	857,675	857,784	815,764	820,019
48,00	858,278	858,574	857,338	857,525	861,516	859,863	848,941	858,194	859,123	859,229	817,189	821,447
46,00	859,723	860,021	858,785	858,971	862,969	861,309	850,500	859,649	860,567	860,677	818,614	822,875
44,00	861,171	861,469	860,231	860,419	864,421	862,757	852,057	861,106	862,015	862,121	820,036	824,300
42,00	862,616	862,917	861,676	861,866	865,873	864,204	853,615	862,564	863,461	863,568	821,460	825,725
40,00	864,062	864,362	863,123	863,315	867,327	865,652	855,172	864,021	864,908	865,014	822,883	827,151
38,00	865,509	865,809	864,570	864,764	868,779	867,100	856,729	865,477	866,356	866,461	824,307	828,574
36,00	866,956	867,257	866,016	866,211	870,232	868,548	858,288	866,933	867,803	867,909	825,728	830,000
34,00	868,403	868,704	867,462	867,659	871,684	869,998	859,843	868,392	869,253	869,355	827,151	831,425
32,00	869,850	870,153	868,910	869,109	873,139	871,446	861,401	869,850	870,700	870,803	828,574	832,849
30,00	871,297	871,600	870,356	870,559	874,593	872,896	862,959	871,308	872,148	872,251	829,992	834,272
28,00	872,747	873,049	871,804	872,007	876,046	874,344	864,516	872,769	873,596	873,702	831,414	835,698
26,00	874,195	874,499	873,253	873,458	877,501	875,795	866,072	874,227	875,047	875,149	832,835	837,121
24,00	875,643	875,949	874,701	874,907	878,958	877,245	867,632	875,688	876,496	876,599	834,256	838,543
22,00	877,092	877,397	876,153	876,359	880,411	878,698	869,188	877,150	877,948	878,051	835,677	839,969
20,00	878,543	878,848	877,601	877,810	881,868	880,149	870,748	878,611	879,400	879,498	837,099	841,392
18,00	879,993	880,300	879,050	879,262	883,327	881,601	872,306	880,072	880,851	880,949	838,520	842,816
16,00	881,446	881,749	880,501	880,714	884,781	883,054	873,867	881,536	882,304	882,399	839,942	844,240

Table C.1 *(continued)*

temp (°C)	PR.1	PR.2	PR.3	PR.4	PR.5	PR.6	PR.7	PR.8	PR.9	PR.10	PR.11	PR.12
14,00	882,897	883,202	881,953	882,167	886,242	884,507	875,430	882,998	883,759	883,853	841,363	845,665
12,00	884,351	884,654	883,403	883,623	887,701	885,965	876,993	884,462	885,211	885,307	842,785	847,090
10,00	885,804	886,107	884,857	885,078	889,159	887,418	878,555	885,930	886,668	886,762	844,205	848,515

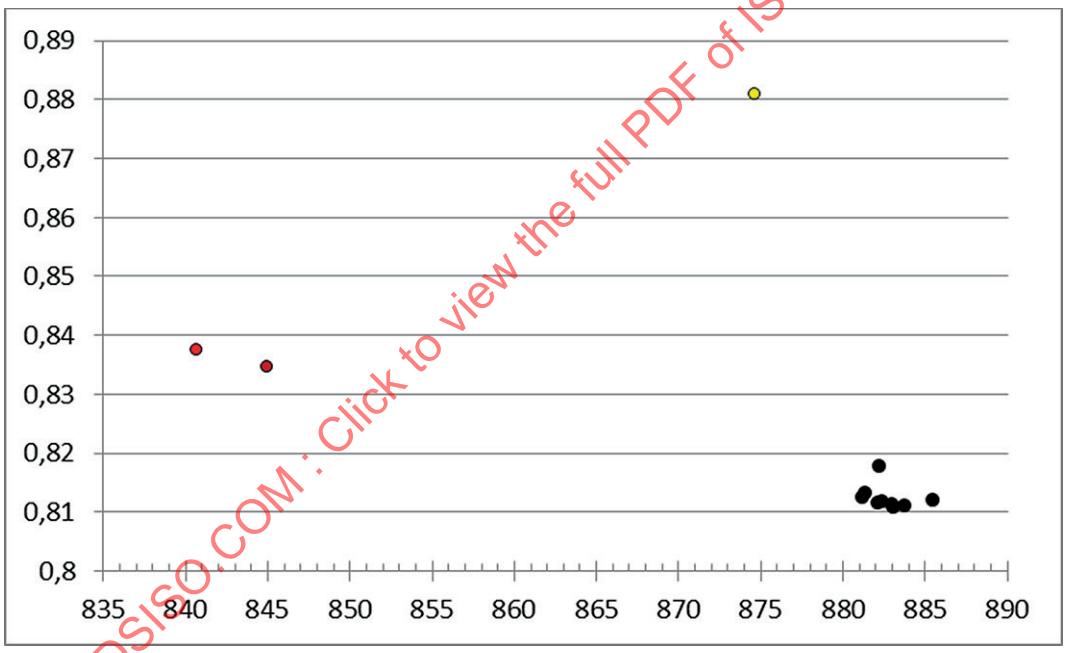
C.3 Additional determination of $D(15)$ and α_{15} for the same 12 FAME samples

In a rather extensive additional measurement campaign the thermal expansion coefficients and densities at 15 °C as well as for 60 °F have been compiled from measurements done on a Parr DSA 5000 instrument, using a sequence of 30 temperatures from 10,00 °C to 70,00 °C. The results for α_{15} and D(15 °C) are shown below in Tables C.2 for those interested. Figure C.2 shows a plot of these data points in α_{15}, $D(15)$ coordinates.

Table C.2 — Results from PMT calculations (exponential model C)

Results from PMT Calculations (Exponent Model "C")

	PR.1	PR.2	PR.3	PR.4	PR.5	PR.6	PR.7	PR.8	PR.9	PR.10	PR.11	PR.12
α(60F)	0,450 89	0,450 9	0,451 31	0,451 8	0,451 1	0,450 5	0,489 5	0,454 3	0,450 7	0,45	0,465 3	0,46 4
D(60F)	881,715	882,02	880,772	880,99	885,05	883,32	874,17	881,81	882,57	882,7	840,23	844,5
α(15C)	0,811 61	0,811 7	0,812 35	0,8132	0,812	0,8109	0,881	0,8177	0,8113	0,811	0,837 6	0,835
D(15C)	882,113	882,42	881,169	881,38	885,45	883,72	874,6	882,21	882,97	883,1	840,62	844,9



Key

X D(15) in kg/m³
Y α_{15} [(* 1 000)]
red diesel fuels B20 and B30
black FAMES of different origins
yellow FAME from coconut oil (CME, sample 7)

Figure C.2 — Plot of data points in α_{15}, $D(15)$ data space

The plot and the tabled values for CME (sample 7) show that CME behaviour is quite different from other members of the FAME product family. Similar differences have also been observed for other lauric FAME products (not discussed here any further).

Annex D
(informative)

Density/temperature tables

This annex presents the density versus temperature data generated following 11.2 for FAME (Tables D.1, D.2 and D.3), FAME blends (Tables D.4, D.7), market distillate fuels and heating oils (Tables D.5, D.6, D.8, D.9, D.10) and oil fuels (Table D.11). For different gasoline/ethanol blends the data are presented in Table D.14 to D.17. As a last information item in this annex, the expansion coefficients for diesel (Table D.13), gasoline blends (Table D.18) and gasoline (Table D.19) are given.

Table D.1 — Density measurement/$D(t)$ evaluation for FAMEs (laboratory A)

Density measurement of 4 FAME samples at 10 temperatures

temp °C	1-RME	2-SOY	3-RME	4-RME
10	886,628	888,748	886,388	886,842
12	885,160	887,278	884,945	885,392
15	882,991	885,101	882,749	883,207
17	881,528	883,638	881,295	881,754
20	879,356	881,456	879,109	879,571
22	877,901	879,994	877,669	878,130
25	875,740	877,826	875,493	875,952
30	872,059	874,144	871,853	872,292
35	868,438	870,533	868,232	868,681
40	864,871	866,875	864,599	865,062

temp °C	1-RME	2-SOY	3-RME	4-RME
10	−0,734	−0,735	−0,721	−0,725
12	−0,723	−0,726	−0,732	−0,728
15	−0,731	−0,731	−0,727	−0,726
17	−0,724	−0,727	−0,729	−0,728
20	−0,728	−0,731	−0,720	−0,721
22	−0,720	−0,723	−0,725	−0,726
25	−0,736	−0,736	−0,728	−0,732
30	−0,724	−0,722	−0,724	−0,722
35	−0,713	−0,732	−0,727	−0,724

	PMT exponent Model				Linear Model	
	α(60F) * 1 000	D(60F) (kg/m^3)	α(15C) * 1 000	D(15C) (kg/m^3)	α(15C) * 1 000	D(15C) (kg/m^3)
1,RME	0,454 94	882,584	0,818 89	882,985	0,822 33	882,986
2,SOY	0,455 59	884,695	0,820 06	885,098	0,823 49	885,099
3,RME	0,455 19	882,351	0,819 34	882,753	0,822 77	882,753
4,RME	0,454 96	882,806	0,818 93	883,208	0,822 36	883,208

Table D.2 — Density measurement/$D(t)$ evaluation for FAMEs (laboratory B)

temp	RME-1a	RME-1b	SOY-1a	SOY-1b	RME-3a	RME-3b	RME-4a	RME-4b
10	886,76	886,76	888,87	888,87	886,41	886,41	886,90	886,90
13	884,78	884,78	886,86	886,86	884,33	884,35	884,83	884,83
15	883,12	883,12	885,23	885,23	882,78	882,78	883,27	883,27
20	879,61	879,61	881,68	881,68	879,24	879,24	879,71	879,71
23	877,43	877,42	879,42	879,42	877,03	877,03	877,50	877,50
25	876,00	876,00	878,06	878,06	875,63	875,63	876,11	876,11
30	872,40	872,40	874,45	874,45	872,02	872,01	872,50	872,49
33	870,26	870,26	872,29	872,29	869,87	869,86	870,34	870,34
35	868,76	868,76	870,79	870,79	868,36	868,36	868,84	868,84
40	865,21	865,21	867,22	867,22	864,81	864,81	865,28	865,28

temp	RME-1a	RME-1b	SOY-1a	SOY-1b	RME-3a	RME-3b	RME-4a	RME-4b
10	−0,66	−0,66	−0,67	−0,67	−0,69	−0,69	−0,69	−0,69
13	−0,83	−0,83	−0,81	−0,81	−0,78	−0,79	−0,78	−0,78
15	−0,70	−0,70	−0,71	−0,71	−0,71	−0,71	−0,71	−0,71
20	−0,73	−0,73	−0,75	−0,75	−0,74	−0,74	−0,74	−0,74
23	−0,71	−0,71	−0,68	−0,68	−0,70	−0,70	−0,69	−0,69
25	−0,72	−0,72	−0,72	−0,72	−0,72	−0,72	−0,72	−0,72
30	−0,71	−0,71	−0,72	−0,72	−0,72	−0,72	−0,72	−0,72
33	−0,75	−0,75	−0,75	−0,75	−0,75	−0,75	−0,75	−0,75
35	−0,71	−0,71	−0,71	−0,71	−0,71	−0,71	−0,71	−0,71

	PMT exponent Model				lin, Model		D15	PMT model	LIN model
							measured	Diff in %	Diff in %
	1 000 * α15	D(60F)	1 000 * α15	D(15C)	1 000 * α15	D(15C)			
RME.1a	0,451 32	882,81	0,812 37	883,21	0,815 70	883,21	883,12	0,010	0,010
RME.1b	0,451 31	882,81	0,812 35	883,20	0,815 69	883,20	883,12	0,009	0,010
SOY.1a	0,452 15	884,89	0,813 87	885,29	0,817 24	885,29	885,23	0,006	0,007
SOY.1b	0,452 15	884,89	0,813 87	885,29	0,817 24	885,29	885,23	0,006	0,007
RME.3a	0,451 95	882,43	0,813 50	882,83	0,816 84	882,83	882,78	0,005	0,005
RME.3b	0,452 20	882,43	0,813 95	882,83	0,817 30	882,83	882,78	0,006	0,006
RME.4a	0,452 14	882,91	0,813 85	883,31	0,817 20	883,31	883,27	0,005	0,005
RME.4b	0,452 18	882,91	0,813 92	883,31	0,817 27	883,31	883,27	0,005	0,005

Table D.3 — Density measurement/$D(t)$ evaluation for FAMEs (laboratory C)

Sample	D(10 °C)	D(15 °C)	D(25 °C)	D(40 °C)
FAME.1a	882,17	885,80	874,91	864,06
FAME.1b	882,17	885,80	874,91	864,06
FAME.2a	882,46	886,10	875,20	864,35
FAME.2b	882,47	886,10	875,21	864,36
FAME.3a	881,22	884,85	873,97	863,13
FAME.3b	881,23	884,86	873,98	863,13
FAME.4a	881,45	885,09	874,19	863,33
FAME.4b	881,46	885,10	874,20	863,34
FAME.5a	885,55	889,20	878,26	867,37
FAME.5b	885,55	889,19	878,26	867,37
FAME.6a	883,73	887,37	876,46	865,60
FAME.6b	883,73	887,37	876,47	865,60
FAME.7a	874,63	878,53	866,83	855,16
FAME.7b	874,63	878,53	866,83	855,16
FAME.8a	882,27	885,93	874,95	864,01
FAME.8b	882,27	885,94	874,95	864,01
FAME.9a	883,07	886,71	875,81	864,94
FAME.9b	883,07	886,71	875,80	864,94
FAME.10a	883,11	886,75	875,85	864,99
FAME.10b	883,12	886,76	875,86	865,00
B.20 a	840,64	844,19	833,54	822,88
B.20 b	840,65	844,20	833,54	822,89
B.30 a	844,90	848,46	837,79	827,11
B.30 b	844,92	848,48	837,80	827,12

	PMT Exponential Model from measurements only at 4 temperatures				**Linear Model from 4 temperatures** (10 °C, 15 °C, 25 °C, 40 °C)			((D(15,meas) – D(15,pred)) /D(15,meas)	
Sample	1 000 * α(60 °F)	D(60 °F)	1 000 * α(15 °C)	D(15 °C)	1 000 * α(15 °C)	D(15 °C)	measured D(15 °C)	Diff zu PMT Model in %	Diff zu LIN Model in %
FAME.1a	0,454 34	881,78	0,817 81	882,18	0,821 46	882,17	882,17	5.67E-04	−1.29E-14
FAME.1b	0,454 34	881,78	0,817 81	882,18	0,821 46	882,17	882,17	5.67E-04	−1.29E-14
FAME.2a	0,454 33	882,07	0,817 80	882,47	0,821 46	882,46	882,46	1.13E-03	4.86E-04
FAME.2b	0,454 18	882,08	0,817 53	882,48	0,821 18	882,47	882,47	5.67E-04	0.00E+00
FAME.3a	0,454 38	880,83	0,817 88	881,23	0,821 53	881,22	881,22	7.94E-04	2.43E-04
FAME.3b	0,454 58	880,84	0,818 25	881,24	0,821 90	881,23	881,23	7.94E-04	2.43E-04
FAME.4a	0,455 06	881,06	0,819 11	881,46	0,822 77	881,45	881,45	1.13E-03	4.86E-04
FAME.4b	0,455 06	881,07	0,819 10	881,47	0,822 77	881,46	881,46	1.13E-03	4.86E-04
FAME.5a	0,454 44	885,16	0,818 00	885,56	0,821 66	885,55	885,55	7.90E-04	2.42E-04
FAME.5b	0,454 30	885,15	0,817 74	885,55	0,821 39	885,55	885,55	3.39E-04	−2.42E-04
FAME.6a	0,454 13	883,34	0,817 43	883,74	0,821 08	883,73	883,73	7.92E-04	2.42E-04
FAME.6b	0,454 10	883,34	0,817 38	883,74	0,821 03	883,73	883,73	1.13E-03	4.85E-04
FAME.7a	0,492 45	874,21	0,886 41	874,64	0,890 66	874,63	874,63	6.86E-04	−1.30E-14
FAME.7b	0,492 45	874,21	0,886 41	874,64	0,890 66	874,63	874,63	6.86E-04	−1.30E-14
FAME.8a	0,458 03	881,87	0,824 46	882,28	0,828 17	882,27	882,27	5.67E-04	0.00E+00
FAME.8b	0,458 18	881,88	0,824 72	882,28	0,828 43	882,27	882,27	1.13E-03	4.86E-04
FAME.9a	0,454 44	882,68	0,817 99	883,08	0,821 64	883,07	883,07	1.13E-03	4.85E-04
FAME.9b	0,454 47	882,68	0,818 04	883,08	0,821 70	883,07	883,07	7.93E-04	2.43E-04
FAME.10a	0,454 21	882,72	0,817 58	883,12	0,821 23	883,11	883,11	1.13E-03	4.85E-04
FAME.10b	0,454 20	882,73	0,817 57	883,13	0,821 22	883,12	883,12	1.13E-03	4.85E-04
B.20 a	0,467 31	840,25	0,841 15	840,65	0,844 99	840,64	840,64	5.95E-04	0.00E+00
B.20 b	0,467 33	840,26	0,841 20	840,65	0,845 04	840,65	840,65	3.57E-04	−2.55E-04
B.30 a	0,465 80	844,51	0,838 44	844,91	0,842 25	844,90	844,90	9.47E-04	2.54E-04
B.30 b	0,466 04	844,53	0,838 86	844,93	0,842 68	844,92	844,92	5.92E-04	0.00E+00

Table D.4 — Density measurement of low sulfur heating oil/FAME blends

$D(T) = A + B * dT + C * X$ (FAME)

A	842,308 2
B	−0,703 81
C	0,392 44

		$D(T)$ in kg/m^3					
Temp. (°C)	(T-15)	FAME 0,05 %(V/V)	FAME 3,0 %(V/V)	FAME 5,0 %(V/V)	FAME 7,0 %(V/V)	FAME 10,2 %(V/V)	FAME 20,1 %(V/V)
10,0	−5,0	845,90	847,00	847,80	848,60	849,80	853,80
10,0	−5,0	845,90	847,00	847,80	848,60	849,80	853,70
15,0	0,0	842,30	843,50	844,20	845,00	846,30	850,20
15,0	0,0	842,30	843,50	844,30	845,00	846,30	850,20
25,0	10,0	835,30	836,50	837,20	838,00	839,20	843,20
25,0	10,0	835,30	836,50	837,20	838,00	839,20	843,20
40,0	25,0	824,70	825,90	826,70	827,50	828,70	832,60
40,0	25,0	824,80	825,90	826,70	827,40	828,70	832,60

For the isolated single blends:

Slope	−0,704 05	−0,703 33	−0,703 10	−0,704 05	−0,703 81	−0,704 52
y-Intercept	842,343	843,500	844,261	845,043	846,279	850,221
1 000 * α_{15}	0,835 82	0,833 83	0,832 79	0,833 15	0,831 65	0,828 64

Table D.5 — Density measurement/$D(t)$ evaluation for diesel fuels (winter grades)

temp	DK-01	DK-02	DK-03	DK-04	DK-05	DK-06	DK-07	DK-08	DK-09	DK-10	DK-11	DK-12	DK-13	DK-14	DK-15	DK-16	DK-17	DK-18	Pr.20
50,00	803,008	814,113	819,061	805,958	818,744	815,945	815,796	802,882	807,157	813,576	807,327	811,160	812,268	810,860	809,885	805,858	812,732	818,255	811,366
45,00	806,530	817,621	822,559	809,483	822,217	819,443	819,341	806,466	810,645	817,111	810,875	814,684	815,833	814,389	813,433	809,385	816,282	821,768	814,893
40,00	810,051	821,129	826,057	813,008	825,720	822,941	822,884	810,053	814,134	820,645	814,422	818,207	819,395	817,917	816,972	812,909	819,825	825,281	818,419
35,00	813,568	824,634	829,553	816,532	829,221	826,438	826,426	813,632	817,623	824,178	817,966	821,728	822,956	821,442	820,506	816,432	823,368	828,791	821,944
30,00	817,081	828,136	833,031	820,048	832,717	829,932	829,960	817,205	821,109	827,687	821,493	825,248	826,514	824,965	824,038	819,953	826,905	832,296	825,464
25,00	820,596	831,638	836,540	823,571	836,217	833,424	833,500	820,779	824,592	831,232	825,045	828,763	830,068	828,487	827,569	823,469	830,444	835,804	828,985
20,00	824,109	835,138	840,028	827,084	839,709	836,916	837,037	824,353	828,070	834,753	828,578	832,281	833,621	832,009	831,102	826,986	833,982	839,313	832,505
15,00	827,622	838,640	843,528	830,605	843,211	840,407	840,574	827,927	831,560	838,284	832,119	835,802	837,178	835,533	834,635	830,508	837,521	842,824	836,027
10,00	831,135	842,144	847,025	834,124	846,711	843,903	844,112	831,498	835,048	841,812	835,658	839,323	840,735	839,060	838,169	834,031	841,062	846,337	839,549
5,00	834,650	845,650	850,523	837,643	850,214	847,399	847,651	835,070	838,536	845,340	839,196	842,847	844,291	842,587	841,705	837,554	844,605	849,854	843,074
0,00	838,169	849,160	854,027	841,166	853,720	850,900	851,192	838,646	842,031	848,873	842,739	846,376	847,854	846,118	845,247	841,079	848,154	853,375	846,602
−5,00	841,698	852,677	857,539	844,695	857,233	854,406	854,741	842,224	845,531	852,412	846,286	849,912	851,421	849,655	848,793	844,610	851,704	856,902	850,136
−10,00	845,723	856,203	861,166	848,248	860,753	858,547	858,543	845,808	849,053	856,519	850,362	854,147	855,442	853,203	852,782	848,712	855,265	860,848	853,968
−15,00	849,862	860,461	865,280	852,553	865,187	862,867	862,688	850,129	853,971	860,825	854,877	858,787	859,573	857,756	856,969	853,082	859,480	865,037	858,309
−20,00	854,093	864,599	869,651	856,687	870,316	867,222	866,914	854,677	859,072	865,297	859,550	863,591	863,724	862,327	861,612	857,542	863,708	869,372	862,782
−25,00	858,545	868,910	874,327	861,022	874,899	871,729	871,304	859,672	864,320	869,951	864,499	868,472	867,992	867,067	866,749	862,111	868,184	873,914	867,420

Results from excponential PMT Model (all temperatures from −25 °C .. 50 °C)

	DK-01	DK-02	DK-03	DK-04	DK-05	DK-06	DK-07	DK-08	DK-09	DK-10	DK-11	DK-12	DK-13	DK-14	DK-15	DK-16	DK-17	DK-18	Pr.20
α (60F)	0,488 54	0,476 43	0,474 94	0,483 38	0,480 46	0,482 02	0,481 39	0,495 32	0,491	0,487 54	0,495 44	0,494 09	0,486 53	0,486 27	0,490 62	0,491 39	0,482	0,479 83	0,485 95
D(60F)	827,659	838,582	843,516	830,547	843,297	840,527	840,545	827,916	831,763	838,389	832,278	836,044	837,169	835,581	834,74	830,626	837,46	842,877	836,086
α (15C)	0,879 38	0,857 57	0,854 88	0,870 08	0,864 83	0,867 64	0,866 5	0,891 58	0,883 79	0,877 56	0,891 79	0,889 37	0,875 75	0,875 29	0,883 12	0,884 5	0,867 6	0,863 69	0,874 71
D(15C)	828,063	838,982	843,917	830,948	843,702	840,932	840,949	828,326	832,172	838,797	832,69	836,457	837,577	835,988	835,149	831,034	837,863	843,281	836,492

Table D.5 *(continued)*

Results from excponential PMT Model (all temperatures from 0 °C .. 50 °C)

	DK-01	DK-02	DK-03	DK-04	DK-05	DK-06	DK-07	DK-08	DK-09	DK-10	DK-11	DK-12	DK-13	DK-14	DK-15	DK-16	DK-17	DK-18	Pr.20
α (60F)	0,469 87	0,462 21	0,458 5	0,468 84	0,459 18	0,460 05	0,465 76	0,477 74	0,463 84	0,465 72	0,470 68	0,465 99	0,470 11	0,466 71	0,468 5	0,469 04	0,467 71	0,460 85	0,466 16
D(60F)	827,261	838,282	843,17	830,243	842,853	840,051	840,21	827,557	831,204	837,92	831,754	835,443	836,813	835,174	834,274	830,149	837,16	842,468	835,666
α(15C)	0,845 77	0,831 98	0,825 3	0,843 91	0,826 53	0,828 08	0,838 37	0,859 92	0,834 91	0,838 29	0,847 22	0,838 78	0,846 19	0,840 08	0,843 31	0,844 27	0,841 88	0,829 53	0,839 08
D(15C)	827,649	838,67	843,556	830,632	843,24	840,437	840,601	827,952	831,59	838,31	832,145	835,832	837,206	835,564	834,665	830,538	837,552	842,856	836,056

Difference between predicted and measured density in %

((A))	0,053	0,041	0,046	0,041	0,058	0,062	0,045	0,048	0,074	0,061	0,069	0,078	0,048	0,054	0,062	0,063	0,041	0,054	0,056
((B))	0,003	0,004	0,003	0,003	0,003	0,004	0,003	0,003	0,004	0,003	0,003	0,004	0,003	0,004	0,004	0,004	0,004	0,004	0,003

Table D.6 — Density measurement/$D(t)$ evaluation for diesel fuels (summer grades)

temp	DK-01	DK-02	DK-03	DK-04	DK-05	DK-06	DK-07	DK-08	DK-10	DK-11	DK-12	DK-13	DK-14	DK-15	DK-16	DK-17	DK-18	Pr.20
50,00	805,295	813,086	817,904	815,038	820,447	813,373	817,362	800,782	819,037	809,494	815,943	808,917	817,361	817,155	816,732	812,513	811,920	813,671
45,00	808,820	816,595	821,388	818,536	823,943	816,865	820,894	804,377	822,529	813,019	819,449	812,471	820,866	820,672	820,267	816,030	815,424	817,187
40,00	812,344	820,102	824,874	822,032	827,440	820,359	824,429	807,968	826,023	816,550	822,954	816,022	824,373	824,190	823,800	819,546	818,930	820,704
35,00	815,864	823,609	828,357	825,529	830,935	823,856	827,959	811,551	829,513	820,073	826,465	819,567	827,872	827,705	827,332	823,057	822,433	824,219
30,00	819,379	827,114	831,840	829,006	834,415	827,343	831,475	815,141	832,995	823,595	829,964	823,115	831,376	831,211	830,852	826,569	825,935	827,729
25,00	822,897	830,615	835,320	832,513	837,916	830,830	835,014	818,724	836,492	827,115	833,464	826,657	834,877	834,730	834,387	830,078	829,433	831,241
20,00	826,413	834,117	838,802	836,003	841,411	834,317	838,541	822,303	839,983	830,634	836,964	830,197	838,377	838,249	837,914	833,586	832,933	834,751
15,00	829,931	837,620	842,287	839,499	844,906	837,806	842,065	825,884	843,472	834,154	840,467	833,741	841,880	841,759	841,443	837,100	836,434	838,263
10,00	833,449	841,124	845,772	842,995	848,401	841,296	845,595	829,464	846,965	837,678	843,971	837,283	845,385	845,273	844,969	840,611	839,937	841,776
5,00	836,969	844,633	849,262	846,493	851,899	844,789	849,127	833,044	850,459	841,202	847,477	840,826	848,891	848,790	848,501	844,126	843,442	845,291
0,00	840,491	848,144	852,757	849,996	855,401	848,285	852,660	836,625	853,960	844,729	850,986	844,372	852,402	852,310	852,036	847,644	846,953	848,810
−5,00	844,363	851,661	856,258	853,505	858,910	852,550	856,200	840,211	858,131	848,736	855,019	848,119	855,920	855,836	855,575	851,572	851,030	852,569
−10,00	848,412	856,127	861,404	857,753	862,774	856,906	860,222	843,800	862,866	853,591	860,000	852,248	860,091	860,034	859,646	855,889	855,391	856,896
−15,00	852,918	860,588	866,469	862,051	867,232	861,696	864,377	847,444	867,170	857,945	864,483	856,260	864,553	864,379	863,920	860,464	860,104	861,297
−20,00	857,449	865,452	870,846	866,851	871,961	866,085	869,019	852,436	871,419	862,389	868,760	860,423	869,481	869,255	868,783	865,498	865,149	865,962
−25,00	861,906	869,847	874,509	871,165	876,121	870,297	873,271	857,570	875,396	866,662	872,564	864,957	873,953	873,844	873,148	870,068	869,714	870,300

PMT - Results Exponential Model T-range -25 °C .. 50 °C

	DK-01	DK-02	DK-03	DK-04	DK-05	DK-06	DK-07	DK-08	DK-10	DK-11	DK-12	DK-13	DK-14	DK-15	DK-16	DK-17	DK-18	Pr.20
α (60F)	0,495 60	0,491 01	0,492 08	0,485 21	0,479 02	0,495 63	0,483 31	0,495 20	0,490 03	0,500 08	0,494 64	0,489 99	0,486 31	0,487 03	0,486 45	0,497 12	0,499 55	0,491 07
D (60F)	830,152	837,872	842,705	839,675	845,009	838,240	842,129	825,816	843,859	834,538	840,880	833,808	842,082	841,938	841,561	837,467	836,884	838,509
α (15C)	0,892 07	0,883 81	0,885 75	0,873 37	0,862 24	0,892 14	0,869 96	0,891 36	0,882 05	0,900 14	0,890 36	0,881 98	0,875 36	0,876 65	0,875 60	0,894 82	0,899 19	0,883 93
D (15C)	830,563	838,283	843,120	840,082	845,414	838,655	842,536	826,225	844,272	834,956	841,296	834,217	842,492	842,348	841,970	837,883	837,302	838,921

Table D.6 *(continued)*

PMT - Results Exponential Model T - range starting 0°C and above

	DK-01	DK-02	DK-03	DK-04	DK-05	DK-06	DK-07	DK-08	DK-10	DK-11	DK-12	DK-13	DK-14	DK-15	DK-16	DK-17	DK-18	Pr.20
α (60F)	0,469 03	0,462 92	0,457 67	0,460 58	0,457 61	0,460 91	0,463 65	0,479 99	0,457 97	0,467 19	0,461 17	0,470 33	0,460 37	0,461 97	0,464 06	0,464 17	0,463 24	0,463 64
D (60F)	829,570	837,262	841,933	839,142	844,548	837,449	841,705	825,513	843,116	833,795	840,109	833,376	841,523	841,398	841,080	836,740	836,077	837,904
α (15C)	0,844 26	0,833 25	0,823 81	0,829 05	0,823 70	0,829 64	0,834 58	0,863 98	0,824 35	0,840 94	0,830 11	0,846 59	0,828 67	0,831 54	0,835 30	0,835 50	0,833 83	0,834 56
D (15C)	829,959	837,650	842,318	839,528	844,934	837,835	842,095	825,909	843,502	834,184	840,497	833,767	841,910	841,787	841,470	837,128	836,464	838,292

Difference between predicted and measured density in %

((A))	0,076	0,079	0,099	0,069	0,060	0,101	0,056	0,041	0,095	0,096	0,099	0,057	0,073	0,070	0,063	0,094	0,104	0,078
((B))	0,003	0,004	0,004	0,003	0,003	0,003	0,004	0,003	0,004	0,004	0,004	0,003	0,004	0,003	0,003	0,003	0,004	0,003

((A)): using the full temperature range including the "instable" region

((B)): using temperatures starting at 0 °C only ("stable" region)

Table D.7 — Density measurement/$D(t)$ evaluation for diesel fuels and corresponding FAME blends

Temp °C	Diesel -S	Diesel -W	B5(RME) -S	B5(RME) -W	B5(SME) -S	B5(SME) -W	B7(RME) -S	B7(RME) -W	B7(SME) -S	B7(SME) -W	RME -S	RME -W	SME -S	SME -W
0,0	855,047	833,227	856,898	836,189	856,976	836,290	857,638	837,365	857,753	837,509	894,257	894,511	896,270	896,652
5,0	851,566	829,710	853,408	832,666	853,486	832,767	854,146	833,840	854,259	833,982	890,601	890,856	892,604	892,984
10,0	848,089	826,196	849,922	829,145	849,999	829,245	850,657	830,317	850,769	830,458	886,954	887,208	888,945	889,324
15,0	844,615	822,682	846,439	825,626	846,515	825,725	847,171	826,795	847,282	826,934	883,314	883,568	885,292	885,671
20,0	841,142	819,169	842,959	822,107	843,034	822,205	843,688	823,274	843,798	823,412	879,681	879,935	881,645	882,024
25,0	837,672	815,655	839,480	818,588	839,555	818,685	840,206	819,752	840,315	819,889	876,054	876,306	878,003	878,381
30,0	834,201	812,140	836,002	815,067	836,075	815,163	836,724	816,229	836,833	816,365	872,430	872,682	874,365	874,742
35,0	830,731	808,622	832,523	811,544	832,596	811,639	833,243	812,704	833,350	812,839	868,810	869,061	870,729	871,106
40,0	827,259	805,101	829,044	808,018	829,115	808,113	829,760	809,176	829,866	809,310	865,192	865,443	867,095	867,472
45,0	823,784	801,576	825,562	804,489	825,633	804,583	826,275	805,644	826,380	805,778	861,575	861,825	863,463	863,838
50,0	820,307	798,047	822,078	800,955	822,148	801,048	822,787	802,108	822,892	802,241	857,958	858,207	859,831	860,204
Results from PMT exponential Model calculation for T range = 0 °C..50 °C														
α (60F)	0,454 93	0,472 92	0,454 99	0,471 96	0,455 06	0,472 02	0,455 01	0,471 60	0,455 08	0,471 67	0,454 46	0,454 40	0,455 23	0,455 13
D (60F)	844,260	822,319	846,085	825,262	846,161	825,361	846,816	826,431	846,927	826,571	882,956	883,210	884,930	885,310
α (15C)	0,818 87	0,851 26	0,818 99	0,849 53	0,819 11	0,849 63	0,819 01	0,848 89	0,819 14	0,849 00	0,818 03	0,817 93	0,819 42	0,819 23
D (15C)	844,644	822,708	846,470	825,652	846,546	825,751	847,201	826,821	847,313	826,961	883,357	883,611	885,333	885,712

Table D.8 — Density measurement/$D(t)$ evaluation for domestic heating oils

Temp °C	HEL03 (S)	HEL05 (S)	HEL06 (S)	HEL08 (S)	HEL11 (S)	HEL15 (S)	HEL16 (S)	HEL17 (S)	HEL18 (S)	HEL03 (W)	HEL05 (W)	HEL08 (W)	HEL17 (W)
50,00	822,554	833,960	821,065	833,467	813,097	817,645	821,558	814,278	817,226	829,972	830,639	833,956	815,588
45,00	826,106	837,529	824,537	837,009	816,639	821,166	825,105	817,803	820,745	833,514	834,228	837,505	819,109
40,00	829,659	841,099	828,009	840,551	820,180	824,685	828,651	821,327	824,264	837,056	837,816	841,053	822,631
35,00	833,208	844,666	831,479	844,091	823,717	828,204	832,196	824,850	827,779	840,591	841,399	844,600	826,149
30,00	836,756	848,231	834,949	847,630	827,254	831,714	835,736	828,353	831,296	844,132	844,978	848,149	829,662
25,00	840,300	851,792	838,416	851,167	830,786	835,231	839,277	831,895	834,805	847,669	848,558	851,691	833,179
20,00	843,845	855,355	841,885	854,705	834,319	838,745	842,817	835,410	838,312	851,206	852,140	855,236	836,695
15,00	847,391	858,919	845,357	858,248	837,851	842,263	846,355	838,930	841,831	854,747	855,722	858,785	840,214
10,00	850,939	862,483	848,828	861,793	841,385	845,780	849,900	842,450	845,347	858,291	859,305	862,338	843,735
5,00	854,489	866,050	852,304	865,342	844,922	849,299	853,444	845,973	848,864	861,839	862,890	865,895	847,259
0,00	858,044	869,622	855,785	868,899	848,464	852,822	856,994	849,501	852,389	865,808	866,480	869,886	850,785
−5,00	862,245	873,196	860,209	874,283	852,861	857,000	861,787	853,914	856,854	870,396	870,073	874,919	854,345
−10,00	866,634	876,776	864,586	879,060	857,278	861,461	866,360	858,333	861,388	875,008	873,673	879,665	858,590
−15,00	871,042	881,012	869,055	883,686	861,951	865,922	870,897	862,869	865,992	879,595	877,808	884,315	863,378
−20,00	874,203	885,037	873,682	888,265	866,787	870,458	875,434	867,446	870,667	884,150	881,866	888,897	867,761
−25,00	878,683	889,114	878,398	892,986	871,224	875,077	879,974	872,121	875,581	888,696	885,932	893,500	872,120
PMT results for Exponential Model temperature range 0 °C .. 50 °C													
α (60F)	0,487 02	0,470 77	0,491 49	0,505 01	0,504 02	0,495 16	0,502 88	0,500 54	0,501 41	0,501 21	0,474 04	0,506 17	0,489 15
D (60F)	847,593	858,806	845,856	859,054	838,334	842,657	846,926	839,392	842,373	855,422	855,591	859,623	840,421
α (15C)	0,876 63	0,847 38	0,884 67	0,909 02	0,907 24	0,891 28	0,905 18	0,900 97	0,902 53	0,902 19	0,853 27	0,911 10	0,880 46
D (15C)	848,006	859,210	846,271	859,487	838,756	843,074	847,352	839,812	842,795	855,851	855,997	860,058	840,832

Table D.9 — Density measurement/$D(t)$ evaluation for low sulfur domestic heating oils (summer grades)

Density Measurements for low sulfur Heating oil (DIN 51503-x) starting at 0 °C **Summer Qualities from the market**

temp	HEL01	HEL02	HEL03	HEL04	HEL05	HEL07	HEL08	HEL10	HEL12	HEL13	HEL14	HEL15	HEL16	HEL17	HEL18
50,00	811,972	825,470	812,715	811,450	833,004	810,521	808,571	820,560	822,343	822,394	818,299	812,843	789,176	808,397	808,404
45,00	815,430	829,026	816,212	814,935	836,491	814,087	812,174	824,055	825,874	825,874	821,853	816,360	792,709	811,893	811,898
40,00	818,890	832,581	819,708	818,420	839,978	817,653	815,775	827,547	829,405	829,355	825,405	819,877	796,241	815,387	815,393
35,00	822,347	836,133	823,203	821,904	843,465	821,216	819,370	831,038	832,934	832,835	828,954	823,392	799,768	818,879	818,884
30,00	825,785	839,683	826,696	825,385	846,936	824,768	822,946	834,507	836,461	836,303	832,500	826,896	803,281	822,360	822,375
25,00	829,258	843,230	830,184	828,864	850,435	828,328	826,562	838,014	839,986	839,795	836,039	830,411	806,820	825,857	825,862
20,00	832,713	846,776	833,681	832,343	853,915	831,882	830,147	841,501	843,510	843,270	839,583	833,921	810,337	829,343	829,350
15,00	836,171	850,324	837,170	835,826	857,410	835,432	833,735	844,992	847,036	846,750	843,127	837,432	813,857	832,828	832,839
10,00	839,629	853,870	840,663	839,316	860,901	838,988	837,324	848,485	850,564	850,229	846,670	840,943	817,377	836,321	836,328
5,00	843,093	857,422	844,160	842,799	864,396	842,543	840,914	851,982	854,094	853,716	850,214	844,457	820,897	839,813	839,821
0,00	846,572	860,977	847,658	846,285	867,897	846,100	844,506	855,480	857,630	857,342	853,763	847,973	824,418	843,308	843,318

PMT Exponential Model calculation results starting at 0 °C

	HEL01	HEL02	HEL03	HEL04	HEL05	HEL07	HEL08	HEL10	HEL12	HEL13	HEL14	HEL15	HEL16	HEL17	HEL18
α (60F)	0,457 61	0,461 84	0,461 68	0,461 01	0,450 15	0,471 01	0,476 71	0,457 10	0,460 76	0,455 53	0,465 21	0,463 99	0,478 94	0,463 63	0,463 67
D (60F)	835,820	849,959	836,813	835,472	857,055	835,067	833,363	844,636	846,676	846,418	842,762	837,072	813,492	832,473	832,482
α (15C)	0,823 70	0,831 31	0,831 03	0,829 83	0,810 27	0,847 83	0,858 07	0,822 78	0,829 37	0,819 95	0,837 37	0,835 18	0,862 10	0,834 53	0,834 60
D (15C)	836,202	850,352	837,199	835,857	857,441	835,461	833,761	845,022	847,066	846,804	843,154	837,460	813,882	832,859	832,868