# Conformity assessment of multicomponent materials or objects: Risk of false decisions due to measurement uncertainty - A case study of denatured alcohols

Elsevier Editorial System(tm) for Talanta
Manuscript Draft

Manuscript Number:

Title: Conformity assessment of multicomponent materials or objects: Risk of false decisions due to measurement uncertainty - a case study of denatured alcohols

Article Type: Research Paper

Keywords: Conformity assessment
Multicomponent object
Measurement uncertainty
Risk of a false decision
Customs control
Denatured alcohols

Corresponding Author: Dr. Ilya Kuselman, D.Sc.

Corresponding Author's Institution: Independent Consultant on Metrology

First Author: Ilya Kuselman, D.Sc.

Order of Authors: Ilya Kuselman, D.Sc.; Francesca Pennecchi, Ph.D.; Ricardo da Silva, Prof.; D. Brynn Hibbert, Prof.

Abstract: Risk of a false decision on conformity of a multicomponent material or object due to measurement uncertainty is discussed. Even if conformity assessment for each component of a material sample is successful, the total probability of a false decision (total consumer's risk or producer's risk) concerning the sample as a whole might still be significant. A model of the total probability of such false decisions is formulated based on the law (theorem) of total probability. It is shown that the total risk can be evaluated as a combination of the particular risks of conformity assessment of sample components. For a more complicated task, i.e. for a larger number of components of a sample under control, the total risk is greater. As a case study, the total probability of false conforming (total consumer's risk) is evaluated for customs control of completely denatured alcohols, where conformity assessment is performed by comparison of chemical analytical test results with the regulatory limits.

Opposed Reviewers:

# Cover letter

Professor Jean-Michel Kauffmann,

Talanta, Editor 11 September, 2016

Dear Prof. Kauffmann,

Please find attached the manuscript by Ilya Kuselman, Francesca Pennecchi, Ricardo J.N.B. da Silva and D. Brynn Hibbert, titled "Conformity assessment of multicomponent materials or objects: Risk of false decisions due to measurement uncertainty – a case study of denatured alcohols", which we would like to publish in Talanta.

This research was supported in part by the International Union of Pure and Applied Chemistry (IUPAC Project 2016-007-1-500).

Best regards,

Dr. Ilya Kuselman,

the manuscript corresponding author,

ilya.kuselman@bezeqint.net

## Novelty Statement

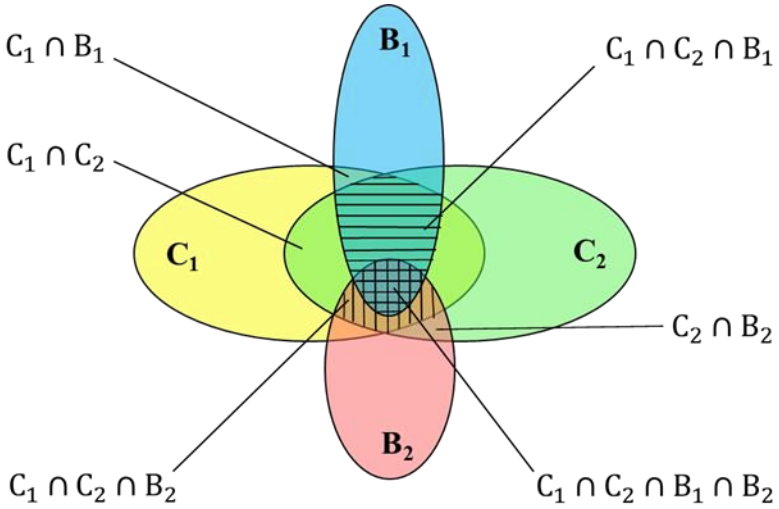
A new model of the risk of false decisions in conformity assessment of a material or object due to measurement uncertainties is formulated based on the law of total probability, allowing the evaluation of the total risk as a combination of the particular risks of conformity assessment of the material components. The customs risks in assessing denatured alcohols are evaluated as a case study.

## Highlights

- Risk of a false decision on compliance of a multicomponent material is studied
- This risk increases with the number of the material components under control
- A new model of the risk is developed based on the law of total probability
- As a case study the risk of customs control of denatured alcohols is evaluated

## Graphical abstract

Venn diagram: events $C_1$ and $C_2$, when test results for components 1 and 2, respectively, are in their acceptance intervals, and events $B_1$ and $B_2$, when the true contents of components 1 and 2 are not actually within their tolerance intervals, are shown by ellipses. Other events of interest are indicated as intersections of these ellipses.



# Conformity assessment of multicomponent materials or objects: Risk of false decisions due to measurement uncertainty – a case study of denatured alcohols

**Ilya Kuselman[a,*] · Francesca Pennecchi[b] · Ricardo J. N. B. da Silva[c] · D. Brynn Hibbert[d]**

[a] Independent Consultant on Metrology, 4/6 Yarehim St., 7176419 Modiin, Israel

[b] Istituto Nazionale di Ricerca Metrologica (INRIM), Strada delle Cacce 91, 10135 Turin, Italy

[c] Faculdade de Ciências da Universidade de Lisboa, Edifício C8, Campo Grande, 1749-016 Lisboa, Portugal

[d] School of Chemistry, UNSW Australia, Sydney NSW 2052, Australia

---

* Corresponding author. Tel.: +972-50-6240466

*E-mail address*: ilya.kuselman@bezeqint.net (I. Kuselman).

4/6 Yarehim St., Modiin, 7176419 Israel

ABSTRACT

Risk of a false decision on conformity of a multicomponent material or object due to measurement uncertainty is discussed. Even if conformity assessment for each component of a material sample is successful, the total probability of a false decision (total consumer's risk or producer's risk) concerning the sample as a whole might still be significant. A model of the total probability of such false decisions is formulated based on the law (theorem) of total probability. It is shown that the total risk can be evaluated as a combination of the particular risks of conformity assessment of sample components. For a more complicated task, i.e. for a larger number of components of a sample under control, the total risk is greater. As a case study, the total probability of false conforming (total consumer's risk) is evaluated for customs control of completely denatured alcohols, where conformity assessment is performed by comparison of chemical analytical test results with the regulatory limits.

**Keywords**

Conformity assessment
Multicomponent object
Measurement uncertainty
Risk of a false decision
Customs control
Denatured alcohols

## 1. Introduction

The JCGM 106 document [1] provides guidance and procedures for assessing conformity of an item (entity, object or system) with specified requirements. The approach of this document is that knowledge about an item property (the measurand) can be treated as a random variable and expressed in terms of a probability density function (pdf). According to Bayes theorem, such a pdf combines prior knowledge of the measurand and new information acquired during the measurement. The posterior pdf provides an estimate of the measurand value and the associated uncertainty, usually taken as the mean and the standard deviation of the distribution, respectively. Comparing this estimate with the limits of the prescribed tolerance interval of the item property values, one should decide whether the tested item conforms or not [2-4]. It is shown that measurement uncertainty influences the decision and causes risks of two types. The probability of accepting the item, when it should have been rejected, is named 'consumer's risk', whereas the probability of falsely rejecting the item is the 'producer's risk'. For a particular tested item, they are the 'specific consumer's risk' and the 'specific producer's risk' [1, Sec. 9.3.2]. The risks of conformity assessment of an item randomly drawn from a statistical population of such items are the 'global consumer's risk' and the 'global producer's risk' [1, Sec. 9.5], since they characterize the item production globally. These risk terms are taken from the field of product manufacture and process control, but they are also applicable in other fields [5].

Besides the tolerance interval, a narrower acceptance interval (i.e. leading to stronger requirements) for the test results can be applied with the purpose of decreasing the consumer's risk by taking into account the measurement uncertainty. In such a case, the decision rules (is the test item conforming or not?) are based on comparing the measured property values with the acceptance limits [1].

Similar procedures are also described in the earlier Eurachem/CITAC guide [6] for chemical analytical testing laboratories, where items of interest are samples for material analysis, customs control, environmental, food or clinical analysis, etc. The tolerance limits for a sample composition are established specifications in the pharmaceutical industry and other industries and fields, regulatory and/or legislative limits, as well as agreed requirements for a non-regulated product under chemical analysis/testing. In current practice, the decision rules are often based on direct comparison of the measured property values with the specification or regulatory limits.

The reason is that these limits have already taken into account the measurement uncertainty, and so the tolerance and the acceptance limits coincide.

Guidance documents [1] and [6] are widely used, for example, for interpretation of test results of spectral analysis of materials [7], conformity assessment of an analytical instrument [8], forensic decisions on blood alcohol content [9], investigation of out-of-specification test results of chemical composition [10], immunochemical screening of blood donors for infectious diseases [11], in legal metrology [12], in numerous calibration and testing laboratories serving industry and trade. These procedures can be applied where the item is characterized by a single scalar quantity (a single measurable property). In other words, the conformity assessment is performed separately for each item property under testing.

The JCGM 106 approach was extended recently for conformity assessment in presence of a systematic measurement error [13], and for qualitative human-based binary nominal and ordinal properties [14, 15]. A multivariate data analysis is described in the EURAMET guide to decision-making and conformity assessment [16] using bivariate examples of the 'post office parcel problem' (limitations of a parcel length and girth) and a healthcare study (skin cream friction and adhesion).

Multivariate conformity assessment is especially important in testing chemical composition of multicomponent materials or objects where measurement uncertainties are not negligible. When conformity assessments for particular components of a sample are successful and *particular* consumer's risks or producer's risks are acceptable, the total probability of a false decision (*total* consumer's risk or producer's risk) on the conformity of the sample as a whole might still be significant. In this regard, a new IUPAC project [17] was started with the purpose of developing guidelines for evaluating the total probability of a false decision in conformity assessment of a multicomponent material or object caused by measurement uncertainties.

In the present position paper of the project, a model for the total probability of a false decision is formulated based on the law (theorem) of total probability [18-20]. As a case study, the total probability of false conforming (total consumer's risk) is evaluated in customs control of denatured alcohols, where conformity assessment is performed by comparison of chemical analytical test results of denaturants content with regulatory limits. Consequences of the risk (financial, safety, quality and/or others) which are important for the risk management [21-23] are not discussed here.

## 2. Modeling

Without losing generality, the proposed modeling is focused just on the consumer's risk. The counterpart model for the total producer's risk is easily obtainable.

### 2.1. *Total global risk*

Define the following events possible during a sample testing, when the test consists in determining content (concentrations) of two sample components:

- $\mathrm{C}_1$: the test result (measured property value) $c_{1\mathrm{m}}$ for component 1 is in its acceptance interval $A_1$; probability of this event is $P(\mathrm{C}_1)$.
- $\mathrm{C}_2$: the test result $c_{2\mathrm{m}}$ for component 2 is in its acceptance interval $A_2$; probability of this event is $P(\mathrm{C}_2)$.
- C: the sample as a whole is accepted, i.e. the test results $c_{1\mathrm{m}}$ and $c_{2\mathrm{m}}$ are in their own acceptance intervals simultaneously, hence $\mathrm{C} = \mathrm{C}_1 \cap \mathrm{C}_2$; probability of this event $P(\mathrm{C}) = P(\mathrm{C}_1)\, P(\mathrm{C}_2)$, if $\mathrm{C}_1$ and $\mathrm{C}_2$ are mutually independent.
- $\mathrm{B}_1$: the true content $c_1$ of component 1 is not within its tolerance interval $T_1$; probability of this event is $P(\mathrm{B}_1)$.
- $\mathrm{B}_2$: the true content $c_2$ of component 2 is not within its tolerance interval $T_2$; probability of this event is $P(\mathrm{B}_2)$.
- B: the sample as a whole is not conforming, i.e. the true content of one or both of the components is not within the corresponding tolerance interval, hence $\mathrm{B} = \mathrm{B}_1 \cup \mathrm{B}_2$; probability of this event is $P(\mathrm{B}) = P(\mathrm{B}_1) + P(\mathrm{B}_2) - P(\mathrm{B}_1 \cap \mathrm{B}_2) = P(\mathrm{B}_1) + P(\mathrm{B}_2) - P(\mathrm{B}_1)\, P(\mathrm{B}_2)$. The last equality is valid if $\mathrm{B}_1$ and $\mathrm{B}_2$ are mutually independent.

Events $\mathrm{C}_1$ and $\mathrm{C}_2$, as well as $\mathrm{B}_1$ and $\mathrm{B}_2$, are shown schematically in Fig. 1 by ellipses of a Venn diagram. Other events of interest are indicated as intersections of these ellipses.

Fig. 1

Particular global consumer's risk $R_{ci}$ for the $i$-th sample component ($i$ = 1, 2) is the probability of false conformance when the corresponding test result falls within its acceptance limits $A_i$, while the true value is outside the tolerance limits $T_i$ :

$$R_{c1} = P(\mathrm{C}_1 \cap \mathrm{B}_1), \quad (1)$$

$$R_{c2} = P(\mathrm{C}_2 \cap \mathrm{B}_2). \quad (2)$$

At the same time, the total global consumer's risk $R_{\mathrm{total}}$ is the risk of having the test results of both the components within their acceptance limits (which are the two-dimensional domain $A_1 \times A_2$), when at least one true content value is outside its tolerance limits $T_1$ and/or $T_2$, i.e. $R_{\mathrm{total}} = \mathrm{C} \cap \mathrm{B}$, where

$$\mathrm{C} \cap \mathrm{B} = \mathrm{C}_1 \cap \mathrm{C}_2 \cap (\mathrm{B}_1 \cup \mathrm{B}_2) = (\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_1) \cup (\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_2). \quad (3)$$

In Fig. 1, event $(\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_1)$ corresponds to the area shaded by horizontal lines, whereas event $(\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_2)$ corresponds to the area shaded by vertical lines. The total global consumer's risk is thus:

$$R_{\mathrm{total}} = P(\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_1) + P(\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_2) - P(\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_1 \cap \mathrm{B}_2). \quad (4)$$

Event $(\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_1 \cap \mathrm{B}_2)$ is marked in Fig. 1 as a net. Whenever $\mathrm{C}_1$ and $\mathrm{C}_2$, as well as $\mathrm{B}_1$ and $\mathrm{B}_2$, are mutually independent, events $\mathrm{C}_1 \cap \mathrm{B}_1$ and $\mathrm{C}_2 \cap \mathrm{B}_2$ are also independent and equation (4) can be rewritten using notations (1) and (2) in the following way:

$$\begin{aligned} R_{\mathrm{total}} &= P(\mathrm{C}_2)P(\mathrm{C}_1 \cap \mathrm{B}_1) + P(\mathrm{C}_1)P(\mathrm{C}_2 \cap \mathrm{B}_2) - P(\mathrm{C}_1 \cap \mathrm{B}_1)P(\mathrm{C}_2 \cap \mathrm{B}_2) \\ &= P(\mathrm{C}_2)R_{c1} + P(\mathrm{C}_1)R_{c2} - R_{c1}R_{c2}. \end{aligned} \quad (5)$$

For example, for particular risks $R_{ci}$= 0.05 and probabilities $P(\mathrm{C}_i)$ = 0.90, formula (5) gives $R_{\mathrm{total}} = 2\times(0.90\times0.05) - 0.05^2 = 0.09$.

For three sample components, under the same assumption of independent true values of each component's content and independent corresponding test results, the total global consumer's risk is:

$$\begin{aligned} R_{\mathrm{total}} = {} & P(\mathrm{C}_2)P(\mathrm{C}_3)R_{c1} + P(\mathrm{C}_1)P(\mathrm{C}_3)R_{c2} + P(\mathrm{C}_1)P(\mathrm{C}_2)R_{c3} - P(\mathrm{C}_3)R_{c1}R_{c2} - \\ & P(\mathrm{C}_2)R_{c1}R_{c3} - P(\mathrm{C}_1)R_{c2}R_{c3} + R_{c1}R_{c2}R_{c3}\,. \end{aligned} \quad (6)$$

For example, for particular risks $R_{ci}$= 0.05 and probabilities $P(\mathrm{C}_i)$ = 0.90, $i$ = 1, 2, 3, formula (6) gives $R_{\mathrm{total}} = 3\times(0.90^2\times0.05) - 3\times(0.90\times0.05^2) + 0.05^3 = 0.12$.

For four components, the total global risk is:

$$R_{\text{total}} = P(\text{C}_2)P(\text{C}_3)P(\text{C}_4)R_{c1} + P(\text{C}_1)P(\text{C}_3)P(\text{C}_4)R_{c2} + P(\text{C}_1)P(\text{C}_2)P(\text{C}_4)R_{c3} + P(\text{C}_1)P(\text{C}_2)P(\text{C}_3)R_{c4} - P(\text{C}_3)P(\text{C}_4)R_{c1}R_{c2} - P(\text{C}_2)P(\text{C}_4)R_{c1}R_{c3} - P(\text{C}_2)P(\text{C}_3)R_{c1}R_{c4} - P(\text{C}_1)P(\text{C}_4)R_{c2}R_{c3} - P(\text{C}_1)P(\text{C}_3)R_{c2}R_{c4} - P(\text{C}_1)P(\text{C}_2)R_{c3}R_{c4} + P(\text{C}_4)R_{c1}R_{c2}R_{c3} + P(\text{C}_3)R_{c1}R_{c2}R_{c4} + P(\text{C}_2)R_{c1}R_{c3}R_{c4} + P(\text{C}_1)R_{c2}R_{c3}R_{c4} - R_{c1}R_{c2}R_{c3}R_{c4}\,. \quad (7)$$

For particular risks $R_{ci}$= 0.05 and probabilities $P(\text{C}_i)$ = 0.90, $i$ = 1, 2, 3, 4, by formula (7) one obtains $R_{\text{total}} = 4\times(0.90^3\times0.05) - 6\times(0.90^2\times0.05^2) + 4\times(0.90\times0.05^3) - 0.05^4 = 0.13$. Comparing this result with the total global risk values for the previous cases of two and three components, it is easy to see that the risk is greater for a larger number of the components under control.

In general, the expression for the total global consumer's risk for a number $n$ of components of a sample under control is:

$$R_{\text{total}} = \sum_{i=1}^{n}\left(\prod_{l\neq i}P(\text{C}_l)\right)R_{ci} - \sum_{i=1}^{n}\sum_{j>i}\left(\prod_{l\neq i,j}P(\text{C}_l)\right)\left(\prod_{q=i,j}R_{cq}\right) + \sum_{i=1}^{n}\sum_{j>i}\sum_{k>j}\left(\prod_{l\neq i,j,k}P(\text{C}_l)\right)\left(\prod_{q=i,j,k}R_{cq}\right) + \cdots + (-1)^{n-2}\sum_{i=1}^{n}P(\text{C}_i)\left(\prod_{q\neq i}R_{cq}\right) + (-1)^{n-1}\prod_{q=1}^{n}R_{cq}\ , \quad (8)$$

where $i$, $j$, $k$, $l$ and $q$ are indices of the sample components in the range (1, … , $n$). Thus, the total global consumer's risk can be evaluated as a combination of $n$ particular global risks of conformity assessment of any material or object in which $n$ components are tested.

## 2.2. *Total specific risk*

When a specific batch is tested concerning content of two components, total specific risk $R^*_{\text{total}}$ is probability $P(\text{B}|c_{1\text{m}}, c_{2\text{m}})$ that the true content of one or both the components in a sample taken from this batch are not within the corresponding tolerance interval ($\text{B} = \text{B}_1 \cup \text{B}_2$), whereas the test/measurement results $c_{1\text{m}}$ and $c_{2\text{m}}$ of both the components are within their acceptance limits.

If the events $\mathrm{B}_1$ and $\mathrm{B}_2$ are conditionally independent [20, p. 57], i.e. independent at the measurement results $c_{1\mathrm{m}}$ and $c_{2\mathrm{m}}$, the total specific risks is

$$R^*_{\mathrm{total}} = P(\mathrm{B}|c_{1\mathrm{m}}, c_{2\mathrm{m}}) = P(\mathrm{B}_1 \cup \mathrm{B}_2|c_{1\mathrm{m}}, c_{2\mathrm{m}}) = P(\mathrm{B}_1|c_{1\mathrm{m}}, c_{2\mathrm{m}}) + P(\mathrm{B}_2|c_{1\mathrm{m}}, c_{2\mathrm{m}}) - P(\mathrm{B}_1 \cap \mathrm{B}_2|c_{1\mathrm{m}}, c_{2\mathrm{m}}) = P(\mathrm{B}_1|c_{1\mathrm{m}}) + P(\mathrm{B}_2|c_{2\mathrm{m}}) - P(\mathrm{B}_1|c_{1\mathrm{m}})P(\mathrm{B}_2|c_{2\mathrm{m}}). \quad (9)$$

Since particular specific consumer's risks $R^*_{ci}$ for the *i*-th component, *i* = 1, 2, are:

$$R^*_{c1} = P(\mathrm{B}_1|c_{1\mathrm{m}}), \quad (10)$$

$$R^*_{c2} = P(\mathrm{B}_2|c_{2\mathrm{m}}), \quad (11)$$

substituting formulas (10) and (11) into formula (9) gives the following:

$$R^*_{\mathrm{total}} = R^*_{c1} + R^*_{c2} - R^*_{c1}R^*_{c2}. \quad (12)$$

For example, for particular specific risks $R^*_{ci} = 0.05$, the total risk by formula (12) is $R^*_{\mathrm{total}} = 2{\times}0.05 - 0.05^2 = 0.10$.

Total specific consumer's risk for three components is:

$$R^*_{\mathrm{total}} = R^*_{c1} + R^*_{c2} + R^*_{c3} - R^*_{c1}R^*_{c2} - R^*_{c1}R^*_{c3} - R^*_{c2}R^*_{c3} + R^*_{c1}R^*_{c2}R^*_{c3}\,. \quad (13)$$

For example, when the particular specific risks are $R^*_{ci} = 0.05$, *i* = 1, 2, 3, the total risk by formula (13) is $R^*_{\mathrm{total}} = 3{\times}0.05 - 3{\times}0.05^2 + 0.05^3 = 0.14$.

When four components are under control, the total specific risk is:

$$R^*_{\mathrm{total}} = R^*_{c1} + R^*_{c2} + R^*_{c3} + R^*_{c4} - R^*_{c1}R^*_{c2} - R^*_{c1}R^*_{c3} - R^*_{c1}R^*_{c4} - R^*_{c2}R^*_{c3} - R^*_{c2}R^*_{c4} - R^*_{c3}R^*_{c4} + R^*_{c1}R^*_{c2}R^*_{c3} + R^*_{c1}R^*_{c2}R^*_{c4} + R^*_{c1}R^*_{c3}R^*_{c4} + R^*_{c2}R^*_{c3}R^*_{c4} - R^*_{c1}R^*_{c2}R^*_{c3}R^*_{c4}\,. \quad (14)$$

For example, when the particular risks are again $R^*_{ci} = 0.05$, *i* = 1, 2, 3, 4, formula (14) gives $R^*_{\mathrm{total}} = 4{\times}0.05 - 6{\times}0.05^2 + 4{\times}0.05^3 - 0.05^4 = 0.19$. Thus, as for the total global risk values, the total specific risk value is greater for a larger number of the components under control.

In general, the total specific consumer's risk for a number *n* of components is:

$$R^*_{\text{total}} = \sum_{i=1}^{n} R^*_{ci} - \sum_{i=1}^{n} \sum_{j>i} \left( \prod_{q=i,j} R^*_{cq} \right) + \sum_{i=1}^{n} \sum_{j>i} \sum_{k>j} \left( \prod_{q=i,j,k} R^*_{cq} \right) + \cdots + (-1)^{n-2} \sum_{i=1}^{n} \left( \prod_{q \neq i} R^*_{cq} \right) + (-1)^{n-1} \prod_{q=1}^{n} R^*_{cq} \,, \quad (15)$$

where *i*, *j*, *k*, *l* and $q$ are indices of the sample components in the range (1, … , *n*).

Note, formulas (5), (6), (7) and (8) for calculation of total global risk can be simplified to similar combinations of the particular global risks as for specific risks in formulas (12), (13), (14) and (15) for 2, 3, 4 and *n* components, respectively, when each probability $P(\mathrm{C}_i)$ of acceptance of the test results for component *i* = 1, 2, …, *n* is equal to 1.

Note also that the model used in the work [24], adopted later in the EURAMET guide [16], defined the total specific risk as one minus the probability that all the involved variables lie within a multivariate 'hyper-rectangle' tolerance region (that is one minus the total conformance probability), seen as the intersection of all the variable particular tolerance regions. When the variables are independent, the total conformance probability is given by the product of the particular conformance probabilities. It can be shown that this model leads to expressions equivalent to formulas (12) - (15) above, hence validating the model proposed in the present work.

### 2.3. *Cases of interdependence of the events*

It is not always possible to assert independence of $\mathrm{C}_1$ and $\mathrm{C}_2$, as well as of $\mathrm{B}_1$ and $\mathrm{B}_2$. A number of chemical analytical techniques are used at method development to overcome possible correlations between measurement results: sample digestion, extraction of analytes from a sample, separation of an analyte from other components, etc. Chemometrics software is applied for separation of spectral signals. Standard additions of an analyte to a sample are used for calibration of a measurement system overcoming multiplicative matrix effects of a sample, and so on. There are requirements in validation guidelines, e.g. [25-27], for evaluating the method selectivity and/or specificity. An experimental proof is necessary that the response of the measurement system is caused by the analyte/component proper, not by another component or

the sample matrix. Still something may happen in practice, but in general this kind of correlation should be negligible.

Correlation of true values of content of different sample components may be caused by stoichiometry of native compounds (in geological, environmental and other samples). The law of conservation of mass means also interdependence of the true concentration values of the components in a sample (their sum must be 100 %). Technological reasons in production of some artificial materials (alloys, drugs, etc.) lead to such correlations as well.

Metrologically-independent test results for two or more components are however inevitably correlated when their true values are correlated. In other words, if $\mathrm{B}_1$ and $\mathrm{B}_2$ are interdependent, also $\mathrm{C}_1$ and $\mathrm{C}_2$ are, though correlation between test results is weaker because of random measurement errors.

For calculating the total consumer's risk taking into account possible correlation between true values of content of components in a sample and/or between results of their measurements, one needs to have the joint pdf of events $\mathrm{C}_i$ and $\mathrm{B}_i$. In such case the last term of expression (4), for example, can be calculated as

$$P(\mathrm{C}_1 \cap \mathrm{C}_2 \cap \mathrm{B}_1 \cap \mathrm{B}_2) = \int_{A_1} \int_{A_2} \int_{T_1} \int_{T_2} g(c_{1\mathrm{m}}, c_{2\mathrm{m}}, c_1, c_2)\, dc_1 dc_2 dc_{1\mathrm{m}}\, dc_{2\mathrm{m}} \ , \qquad (16)$$

where $g$ is a multivariate pdf of measured values $c_{1\mathrm{m}}$ and $c_{2\mathrm{m}}$ and true values $c_1$ and $c_2$ of content of components 1 and 2, respectively.

In the Bayesian context [1], the joint pdf can be rewritten as $g(c_{1\mathrm{m}}, c_{2\mathrm{m}}, c_1, c_2) = h(c_{1\mathrm{m}}, c_{2\mathrm{m}}|c_1, c_2)\, g_0(c_1, c_2)$, where $h$ is a bivariate pdf of measured values $c_{1\mathrm{m}}$ and $c_{2\mathrm{m}}$, taking into account possible correlation between them, when the true values are $c_1$ and $c_2$ (likelihood), whereas $g_0$ is a bivariate pdf of true values $c_1$ and $c_2$ (prior to measurements). Often, as the likelihood, a bivariate normal distribution can be used, having as expectation the mean vector $[c_1, c_2]$ and as covariance matrix the measurement uncertainty matrix:

$$\begin{bmatrix} u^2(c_{1\mathrm{m}}) & u(c_{1\mathrm{m}}, c_{2\mathrm{m}}) \\ u(c_{1\mathrm{m}}, c_{2\mathrm{m}}) & u^2(c_{2\mathrm{m}}) \end{bmatrix}, \qquad (17)$$

where $u(c_{i\mathrm{m}})$ is the standard uncertainty of the $i$-th measurement result, and $u(c_{1\mathrm{m}}, c_{2\mathrm{m}})$ is the covariance between the two.

Principal component analysis (PCA) of the observed multivariate data can be employed to handle effects of covariance on conformance probabilities, as shown in a study of skin cream friction and adhesion described in Deliverable 3.2.4 of the EURAMET guide [16] and references therein.

## 3. Evaluation of the risks in customs control of denatured alcohols caused by measurement uncertainty

The guidelines of World Customs Organization [28] and European Commission [29, 30] define risk as the potential non-compliance with customs laws. Risk analysis in customs control includes the systematic use of available information to determine how often the defined event may occur, i.e. its likelihood or probability. When substances and/or materials are under customs control, one of such risks is caused by measurement uncertainty of chemical analytical test results.

For example, alcohol (ethanol for human consumption) is subject to excise duties, while denatured alcohols (for industrial use) are not, and the task of the control is to distinguish between them [31]. According to EU Regulation [32], a common procedure for the purpose of completely denaturing alcohol consists of addition of 3 L of isopropyl alcohol (IPA), 3 L of methyl ethyl ketone (MEK) and of 1 g of denatonium benzoate (DB) to 100 L (1 hL) of absolute ethyl alcohol (EtOH). Similar regulations exist in Israel [33], Australia [34] and other countries.

Analytical methods for testing completely denatured alcohol (CDA) include determination of EtOH, IPA and MEK using gas chromatography with flame ionization detection (GC-FID) and determination of DB using high performance liquid chromatography with ultraviolet detection (HPLC-UV). The analytes are separated completely from other components of a sample at the chromatographic conditions of the methods. Relevant internal standards and calibration standards are used for quantification of the analyte concentrations. IPA and MEK concentrations are expressed in L per hL of EtOH (as measured), DB concentration – in g per hL of EtOH. These methods have been recently validated at the Institute for Reference Materials and Measurements (IRMM) with participation of a number of customs laboratories [35]. There is no

evidence of correlation between measured values of the measurands. The standard measurement uncertainties were evaluated in the validation process based on the interlaboratory study: $u_1$ = 0.05 L·hL$^{-1}$ for IPA, $u_2$ = 0.07 L·hL$^{-1}$ for MEK, and $u_3$ = 0.07 g·hL$^{-1}$ for DB. As the measurand is the denaturant concentration in a batch of alcohol, the variation of test results is influenced by inhomogeneity of the batches also [36]. Moreover, the contribution of inhomogeneity is dominant here. Therefore, in practice the following relative standard deviations of test results are set in the report [35] as acceptable: 5 % or $s_{r1} = s_{r2} = 0.05$ in fractions of 1for IPA and MEK, and 10 % or $s_{r3} = 0.10$ for DB.

A decision on conformity assessment can be made using IPA and MEK test results, rather than DB test results [35]. Therefore, an analysis of the customs' risks caused by the measurement uncertainties is discussed below for the two scenarios: when IPA and MEK concentrations only are under control, and when concentrations of all the denaturants (IPA, MEK and DB) are considered. Since the customs authority dealing with CDA is the 'consumer' in this study, the customs' risks caused by the measurement uncertainties are the consumer's risks.

### 3.1. *Evaluation of the total global customs risk*

Because denaturing is the process of transformation of absolute ethanol into an undrinkable poisonous mixture of chemicals, the regulatory requirements to the true concentrations $c_1$, $c_2$ and $c_3$ of the denaturants, IPA, MEK and DB, respectively, are the single lower regulatory limits $lrl_1$, $lrl_2$ and $lrl_3$ of their tolerance intervals. By regulation [32], IPA and MEK concentrations $c_1$ and $c_2$ in a CDA sample shall be not less than $lrl_1 = lrl_2 = 3$ L·hL$^{-1}$, whereas DB concentration $c_3$ - not less than $lrl_3 = 1$ g·hL$^{-1}$.

The $i$-th particular global customs risk, $i$ = 1, 2, 3, can be evaluated by the following formulas [1, 10]:

$$R_{ci} = \int_0^{lrl_i} \int_{lal_i}^{\infty} f(c_{i\mathrm{m}}|c_i) f(c_i)\, \mathrm{d}c_{im} \mathrm{d}c_i, \tag{18}$$

where $lal_i$ is the lower acceptance limit for the measurement/test results $c_{i\mathrm{m}}$, $f(c_i)$ is the pdf of the global distribution of $c_i$ values (the prior pdf), and $f(c_{i\mathrm{m}}|c_i)$ is the pdf of the distribution of measurement results $c_{i\mathrm{m}}$ when the true value is $c_i$ (the likelihood function). The lower bound of the outer integral is equal to zero, since concentration of a denaturant is a non-negative property.

The standard measurement uncertainties $u_i$ can be applied as the standard deviations of the distribution of measurement results $c_{i\mathrm{m}}$. When a customs laboratory database contains a statistically significant number of test results of CDA batches, the global distribution of true $c_i$ values can be approximated by an empirical distribution of these 'batch-to-batch' results as shown in the Guide [10]. In the current case study the relative standard deviations $s_{ri}$, taking into account inhomogeneity of the batches, are used for calculating the standard deviations of the global distributions. For simplicity the global distributions are approximated by the following normal distributions:

$$f(c_i) = \frac{1}{s_{\mathrm{r}i}\mu_i\sqrt{2\pi}} \exp\left[-\frac{(c_i - \mu_i)^2}{2(s_{\mathrm{r}i}\mu_i)^2}\right], \tag{19}$$

where $\mu_i$ is the mean, and $s_i\mu_i$ is the standard deviation of the global distribution. The measurement distributions (likelihood functions) are taken as normal as well:

$$f(c_{i\mathrm{m}}|c_i) = \frac{1}{u_i\sqrt{2\pi}} \exp\left[-\frac{(c_{im} - c_i)^2}{2u_i^2}\right]. \tag{20}$$

In order to apply formula (18), normal distributions truncated at zero should be used both for the prior and the likelihood pdfs, however, for the example under consideration the influence of the truncation is negligible. The results of calculations of the particular global risks $R_{ci}$ in dependence on $\mu_i$ values, when a measurement/test result is compared directly with the regulation limit ($lal_i$ = $lrl_i$), are presented in Fig. 2 for IPA and MEK, curves 1 and 2, respectively, and in Fig. 3 - for DB. From Fig. 2, one can notice how greater measurement uncertainties lead to greater risks. For example, in this study at $\mu_1$ = $\mu_2$ = 3.15 L·hL$^{-1}$ and $\mu_3$ = 1.10 g·hL$^{-1}$ the following risks are observed: $R_{c1}$= 0.027 for IPA and $R_{c2}$ = 0.034 for MEK at, and $R_{c3}$ = 0.046 for DB. They are indicated by dotted lines 3 and 4 for IPA, and 5 and 6 for MEK in Fig. 2; and by dotted lines 2 and 3 for DB in Fig. 3.

Fig. 2

Fig. 3

The probability $P(\mathrm{C}_i)$ of acceptance of a measurement/test results for *i*-th denaturant is calculated by marginalization of the corresponding joint pdf:

$$P(\mathrm{C}_i) = \int_0^{\infty} \int_{lal_i}^{\infty} f(c_{i\mathrm{m}}|c_i) f(c_i)\, \mathrm{d}c_{im} \mathrm{d}c_i \,. \tag{21}$$

The following results were obtained (again at $lal_i = lrl_i$) when $\mu_1 = \mu_2 = 3.15$ L·hL$^{-1}$ and $\mu_3 = 1.10$ g·hL$^{-1}$: $P(\mathrm{C}_1) = 0.818$ for IPA, $P(\mathrm{C}_2) = 0.808$ for MEK, and $P(\mathrm{C}_3) = 0.778$ for DB.

The total global customs risk, in the case of control of IPA and MEK at the above mentioned conditions, is given by formula (5): $R_{\mathrm{total}} = 0.808\times0.027 + 0.818\times0.034 - 0.027\times0.034 = 0.048$. It is greater than each particular risk.

When all the three denaturants (IPA, MEK and DG) are under control at the same conditions, the total global customs risk by formula (6) is $R_{\mathrm{total}} = 0.808\times0.778\times0.027 + 0.818\times0.778\times0.034 + 0.818\times0.808\times0.046 - 0.778\times0.027\times0.034 - 0.808\times0.027\times0.046 - 0.818\times0.034\times0.046 + 0.027\times0.034\times0.046 = 0.066$. This value is greater than that calculated in the case of control on just IPA and MEK.

### 3.2. *Evaluation of the total specific customs risk*

When a specific CDA batch is under customs control, the particular specific customs risk value $R_{ci}^*$ for the *i*-th denaturant can be evaluated according to JCGM 106 [1, Sec. A]:

$$R_{ci}^* = \int_0^{lrl_i} f(c_i|c_{im})\, \mathrm{d}c_i \,, \tag{22}$$

where

$$f(c_i|c_{im}) = \frac{1}{u_{i\mathrm{Post}}\sqrt{2\pi}} \exp\left[-\frac{(c_i - \mu_{i\mathrm{Post}})^2}{2{u_{i\mathrm{Post}}}^2}\right] \tag{23}$$

is the posterior pdf for the true values of the *i*-th denaturant concentration $c_i$, while the measurement result obtained at the batch testing is $c_{i\mathrm{m}}$. When both the prior and likelihood are normal distribution, also the posterior pdf is normal with the following parameters:

$$\mu_{i\mathrm{Post}} = \frac{{\mu_i}/{(s_{\mathrm{r}i}\mu_i)^2} + {c_{i\mathrm{m}}}/{{u_i}^2}}{{1}/{(s_{\mathrm{r}i}\mu_i)^2} + {1}/{{u_i}^2}} \,, \tag{24}$$

$$u_{i\mathrm{Post}} = \frac{1}{\sqrt{1/(s_{\mathrm{r}i}\mu_i)^2 + 1/u_i^2}}. \qquad (25)$$

The $R^*_{ci}$ values calculated at the same conditions as in the previous section ($\mu_1$ = $\mu_2$ = 3.15 L·hL$^{-1}$ and $\mu_3$ = 1.10 g·hL$^{-1}$), in dependence on measurement results $c_{i\mathrm{m}}$ within their acceptance interval, are shown in Fig. 4 by lines 1 and 2 for IPA and MEK, respectively; for DB – in Fig. 5 by line 1.

For example, when a customs laboratory reports in a certificate of analysis of a CDA batch the test results $c_{1m}$= 3.10 L·hL$^{-1}$ for IPA, also $c_{2m}$= 3.10 L·hL$^{-1}$ for MEK, and $c_{3m}$= 1.05 g·hL$^{-1}$ for DB, the batch should be recognized as properly denatured according to the regulation [32]. However, there are still the following particular specific customs risks: $R^*_{c1}$= 0.014, $R^*_{c2}$= 0.045, and $R^*_{c3}$= 0.138. They are shown by dotted lines 3 and 4 for IPA, 5 and 6 for MEK in Fig. 4, and by dotted lines 2 and 3 for DB in Fig. 5. If IPA and MEK only influence the decision on the batch conformity, the total specific risk is $R^*_{\mathrm{total}}$ = 0.014 + 0.045 – 0.014×0.045 = 0.059, by formula (12). When all the denaturants are taken into account, the total specific risk is $R^*_{\mathrm{total}}$ = 0.014 + 0.045 + 0.138 – 0.014×0.045 – 0.014×0.138 – 0.045×0.138 + 0.014×0.045×0.138 = 0.188, by formula (13). This value is caused mostly by DB, since $R^*_{c3}$ is significantly larger here than $R^*_{c1}$ and $R^*_{c2}$. At the same time, consequences of the risk related to the DB concentration are probably less important than other ones, inasmuch as DB is the bitterest chemical compound known and some variations of its concentration do not change the terrible bitter feeling of a person trying to drink CDA. However, this topic is out of the aim of the current study.

Fig. 4

Fig. 5

## 4. Conclusion

When separate conformity assessment for each component of a multicomponent material or object is successful, the total probability of a false decision (consumer's risk or producer's risk) concerning the conformity of the material or object as a whole may still be significant. This probability, caused by measurement uncertainties, is larger for a more complicated composition,

i.e. for a greater number of components of the material or object. Mutual correlations of concentrations of the components can influence the risk value.

A model for the total probability of false conforming (consumer's risk) based on the law of total probability is developed. This model is helpful for evaluation of the total global consumer's risk as a combination of particular global risks of any number of the components under control. Evaluation of the total specific risk as a combination of the particular specific risks is also possible based on this model.

Analysis of such risks in customs control of completely denatured alcohols is detailed as a case study.

## Acknowledgement

This research was supported in part by the International Union of Pure and Applied Chemistry (IUPAC Project 2016-007-1-500).

## References

[1] BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML, Joint Committee for Guidesin Metrology - JCGM 106:2012, Evaluation of Measurement Data – The Role of Measurement Uncertainty in Conformity Assessment (2012), www.bipm.org/en/publications/

[2] I. Lira, A Bayesian approach to the consumer's and producer's risks in measurement, Metrologia 36 (1999) 397–402

[3] G.B. Rossi and F. Crenna, A probabilistic approach to measurement-based decisions, Measurement 39 (2006) 101–119

[4] A.B. Forbes, Measurement uncertainty and optimized conformance assessment, Measurement 39 (2006) 808–814

[5] W.T. Estler and D.B. Hibbert, JCGM 106:2012 – A new guidance document on measurement uncertainty and conformity assessment. OIML Bulletin LIV/2 (2013)14-16

[6] S.L.R. Ellison and A. Williams (eds), EURACHEM/CITAC Guide: Use of Uncertainty Information in Compliance Assessment (2007), www.eurachem.org

[7] Thermo Scientific, Measurement Uncertainty and Material Conformance Probability. Standard OXSAS software feature for Thermo Scientific OES and XRF spectrometers (2012), https://tools.thermofisher.com/content/sfs/brochures/XO-PS41282-OXSAS-Measurement-Uncertainty-1112.pdf

[8] G.V. Hoyos and G.G. Horta, Conformity assessment of a HPLC calibration. In: 16th International Congress of Metrology, DOI: 10.1051/metrology/201305003 (2013), http://cfmetrologie.edpsciences.org/articles/metrology/pdf/2013/01/metrology_metr2013_05003.pdf

[9] L. Zamengo, G. Frison, G. Tedeschi et al. Variability of blood alcohol content (BAC) determinations: The role of measurement uncertainty, significant figures, and decision rules for compliance assessment in the frame of a multiple BAC threshold law, Drug Testing and Analysis 6/10 (2014) 1028-1037

[10] I. Kuselman, F. Pennecchi, C. Burns, A. Fajgelj, P. de Zorzi, IUPAC/CITAC Guide: Investigating out-of-specification test results of chemical composition based on metrological concepts (IUPAC Technical Report). Pure Appl. Chem. 84 (2012) 1939-1971

[11] P. Pereira, B. Magnusson, E. Theodorsson, J. O. Westgard, P. Encarnação, Measurement uncertainty as a tool for evaluating the 'grey zone' to reduce the false negatives in immunochemical screening of blood donors for infectious diseases. Accred. Qual. Assur. 21(2016) 25-32

[12] OIML Document Draft: The role of measurement uncertainty in conformity assessment decisions in legal metrology (2015), https://www.gov.uk/government/uploads/system/uploads/attachment_data/file/503515/TC3_SC5_P2_DD_Uncertainty_clean.pdf

[13] C. Carobbi and F. Pennecchi, Bayesian conformity assessment in presence of systematic measurement errors, Metrologia 53(2016) S74-S80L

[14] L. Pendrill Using measurement uncertainty in decision-making and conformity assessment, Metrologia 51(2014) S206-S218

[15] L. Pendrill and N. Petersson, Metrology of human-based and other qualitative measurements, Meas. Sci. Technol. 27/9 (2016) DOI:10.1088/0957-0233/27/9/094003

[16] L. Pendrill, H. Karlson, N. Fischer, S. Demeyer, A. Allard, EURAMET: A guide to decision-making and conformity assessment - A report of the EMRP joint project NEW04

"Novel mathematical and statistical approaches to uncertainty evaluation" (2015), http://publikationer.extweb.sp.se/ViewDocument.aspx?RapportId=29488

[17] IUPAC Project 2016-007-1-500 Risk of conformity assessment of multicomponent material or object in relation to measurement uncertainty of its test results (2016), http://iupac.org/project/2016-007-1-500

[18] D. Rumsey, Probability for Dummies. Wiley (2006), ISBN 978-0-471-75141-0, p. 58

[19] K. Baclawski, Introduction to Probability with R. CRC Press (2008), ISBN 978-1-4200-6521-3, p. 179

[20] H. Pishro-Nik, Introduction to Probability, Statistics and Random Processes, Kappa Research LLC (2014), ISBN 978-0-9906372-0-2, p. 51

[21] ISO Guide 73, Risk management — Vocabulary. ISO (2009), Geneva

[22] ISO 31000, Risk management — Principles and guidelines. ISO (2009), Geneva

[23] IEC/ISO 31010, Risk management — Risk assessment techniques. ISO (2009), Geneva

[24] A. Subaric-Leitis, Risikoanalyse multivariater Konformitätsprüfungen. tm - Technisches Messen 77 (2010) 662-670

[25] B. Magnusson and U. Ornemark (eds), Eurachem Guide: The Fitness for Purpose of Analytical Methods – A Laboratory Guide to Method Validation and Related Topics (2014), 2nd ed.

[26] ICH Harmonized Tripartite Guideline Q2(R1), Validation of Analytical Procedures. Text and Methodology (2005)

[27] A. Kruve , R. Rebane , K. Kipper , M.L. Oldekop , H. Evard , K. Herodes , P. Ravio , I. Leito, Tutorial review on validation of liquid chromatography-mass spectrometry methods: part I and part II. Anal Chim Acta 870 (2015) 8-28 and 29-44

[28] World Customs Organization, Risk management guide (2003), http://doca.mof.gov.tw/public/Attachment/9581611756.pdf

[29] European Commission, Customs Policy Committee, A guide to risk analysis and customs control (1999), http://biblio.central.ucv.ro/bib_web/bib_pdf/EU_books/0070.pdf

[30] European Commission, Directorate General, Taxation and Customs Union, Risk management guide for tax administrations (2010), http://ec.europa.eu/taxation_customs/resources/documents/common/publications/info_docs/taxation/risk_managt_guide_en.pdf

[31] I. Kuselman, B. Ginzburg, O. Dreazen, Risk analysis in customs control: conformity assessment of denatured alcohols using measurement uncertainty evaluation. In: Isranalytica Conference and Exhibition, Jan 19-20, 2016, Tel Aviv, Israel, https://bioforumconf.com/isranalytica-abs/outofhtml/isranalytica_2016/riskanalysisi_Ilya_Kuselman.html

[32] Commission implementing regulation (EU) 162/2013 amending the Annex to Regulation (EC) No. 3199/93 on the mutual recognition of procedures for the complete denaturing of alcohol for the purposes of exemption from excise duty, http://eur-lex.europa.eu/LexUriServ/ LexUriServ.do?uri=OJ:L:2013:049:0055:0061:EN:PDF

[33] Israel Regulations of Denatured Alcohols (1932), http://www.nadel-law.co.il/Index.asp?ArticleID=642&CategoryID=231

[34] Australian Government, Australian Taxation Office, The Alcohol Industry - Excise Technical Guidelines (2006), www.ato.gov.au/law/view/document?docid=SAV/ALCIND/00009 &PiT=99991231235958

[35] E. Aries, F. Cordeiro, A. Maquet, A. Boix, B. Slowikowski, C. Von Holst, Euro-denaturant project – Phase II, Administrative Arrangement TAXUD-2014-DE-317, Geel, Belgium, European Commission, Joint Research Centre – Institute for Reference Materials and Measurements, JRC101833 (2016), 70 pp

[36] M.H. Ramsey and S.L.R Ellison (eds), Eurachem/CITAC Guide: Measurement uncertainty arising from sampling. A guide to methods and approaches (2007), www.eurachem.org

**Figure captions**

**Fig. 1. Venn diagram of the considered events**. Events $C_1$ and $C_2$, when test results for components 1 and 2, respectively, are in their acceptance intervals, and events $B_1$ and $B_2$, when the true contents of components 1 and 2 are not actually within their tolerance intervals, are shown by ellipses. Other events of interest are indicated as intersections of these ellipses: $C_1 \cap C_2$ – test results for both components 1 and 2 being in their acceptance intervals simultaneously; $C_1 \cap B_1$ and $C_2 \cap B_2$ – test results for component 1 or 2, respectively, being in its acceptance interval, whereas corresponding true contents are not actually within their tolerance interval; $C_1 \cap C_2 \cap B_1$ and $C_1 \cap C_2 \cap B_2$ – test results for both components 1 and 2

being in their acceptance intervals simultaneously, when the true content of component 1 or 2, respectively, is not actually within its tolerance interval; $C_1 \cap C_2 \cap B_1 \cap B_2$ – test results for both components 1 and 2 being in their acceptance intervals, when none of the true contents of the components are within their tolerance intervals.

**Fig. 2. Particular global customs risks $R_{ci}$ at control of IPA and MEK concentrations.** Curve 1 is for IPA ($i$ = 1), and curve 2 – for MEK ($i$ = 2); $\mu_i$ is the mean of the global distribution of true values of the denaturant concentrations $c_1$ and $c_2$ in CDA batches. The risk values at $\mu_1 = \mu_2 =$ 3.15 L·hL$^{-1}$ are indicated by dotted lines 3 and 4 for IPA, and dotted lines 5 and 6 for MEK.

**Fig. 3. Particular global customs risk $R_{c3}$ at control of DB concentrations.** $\mu_3$ is the mean of the global distribution of true DB concentrations $c_3$ in CDA batches. The risk value at $\mu_3 = 1.10$ g·hL$^{-1}$ is indicated by dotted lines 2 and 3.

**Fig. 4. Particular specific customs risk $R^*_{ci}$ at control of IPA and MEK concentrations.** Line 1 is for IPA ($i$ = 1), and line 2 – for MEK ($i$ = 2); $c_{\text{im}}$ is the measurement result value. Dotted lines 3 and 4 mark an example for IPA, 5 and 6 – for MEK.

**Fig. 5. Particular specific customs risk $R^*_{c3}$ at control of DB concentrations.** Line 1 is the dependence of the risk on the concentration measurement result $c_{3\text{m}}$. Dotted lines 2 and 3 indicate an example.

# Checklist

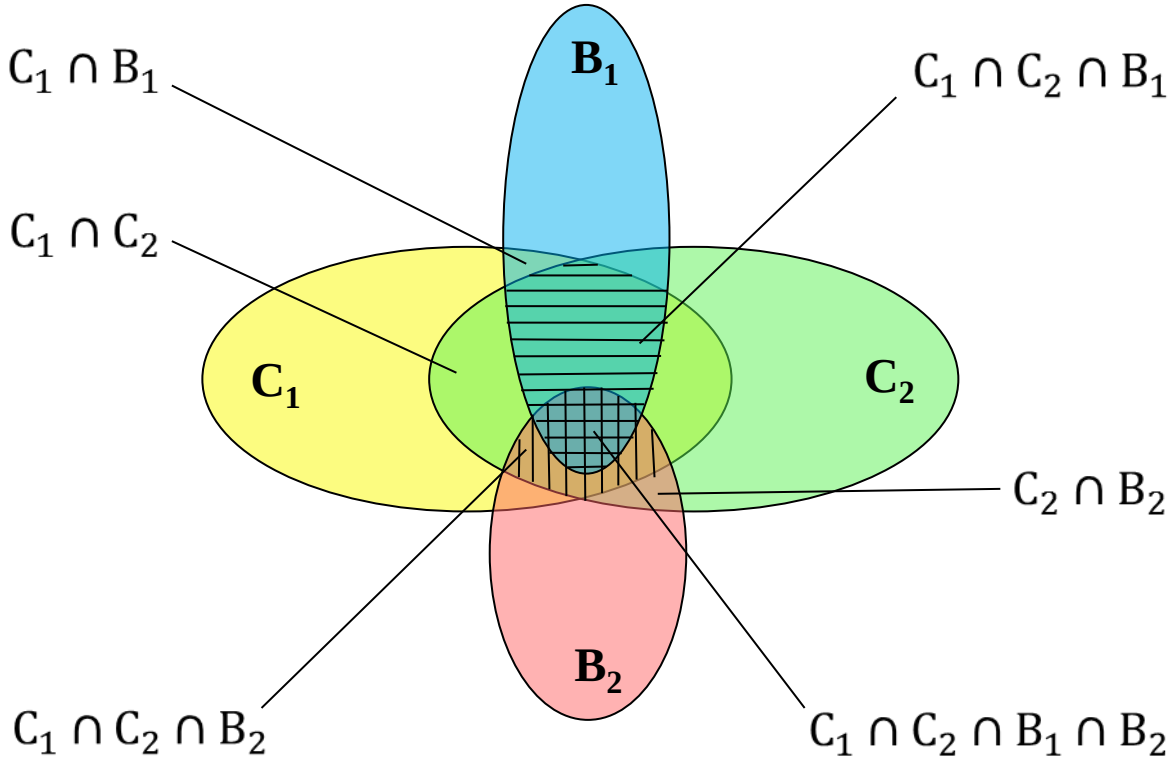
1. Cover Letter
2. Novelty Statement
3. Highlights
4. Manuscript
5. Figures
6. Checklist
7. List of Three Potential Reviewers

***List of Three Potential Reviewers**

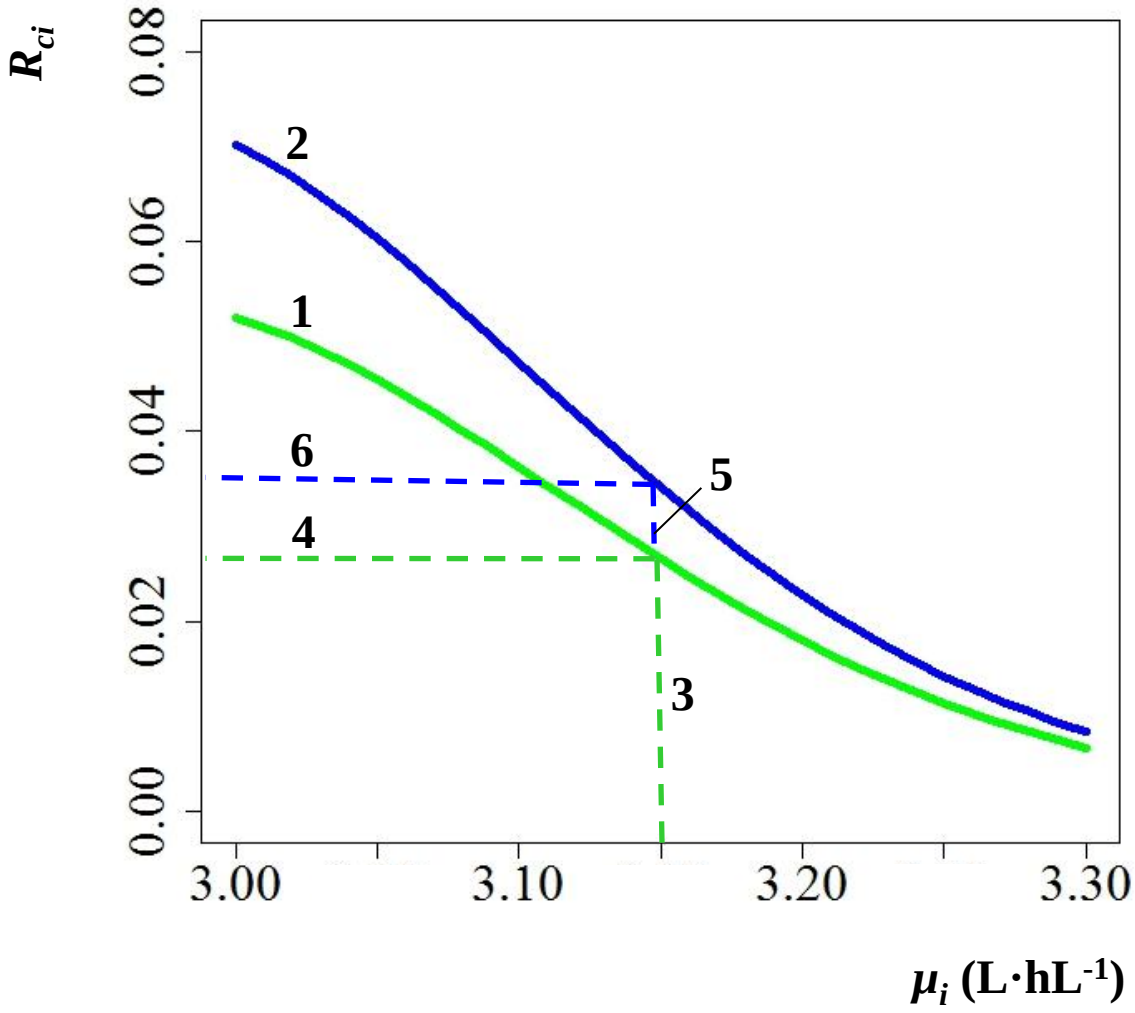
**Possible reviewers**

1. Prof. Wolfhard Wegscheider, Eurachem Chair, Faculty of General and Analytical Chemistry, University of Leoben, Austria, wolfhard.wegscheider@unileoben.ac.at
2. Dr. Della W.M. Sin, Government Chemist, Government Laboratory, Hong Kong, P. R. China, wmsin@govtlab.gov.hk
3. Dr. Boris Ginzburg, Senior Chief Coordinator Commodity Classification, Department of Customs & Vat, Tax Authority, Israel, BorisGi2@taxes.gov.il

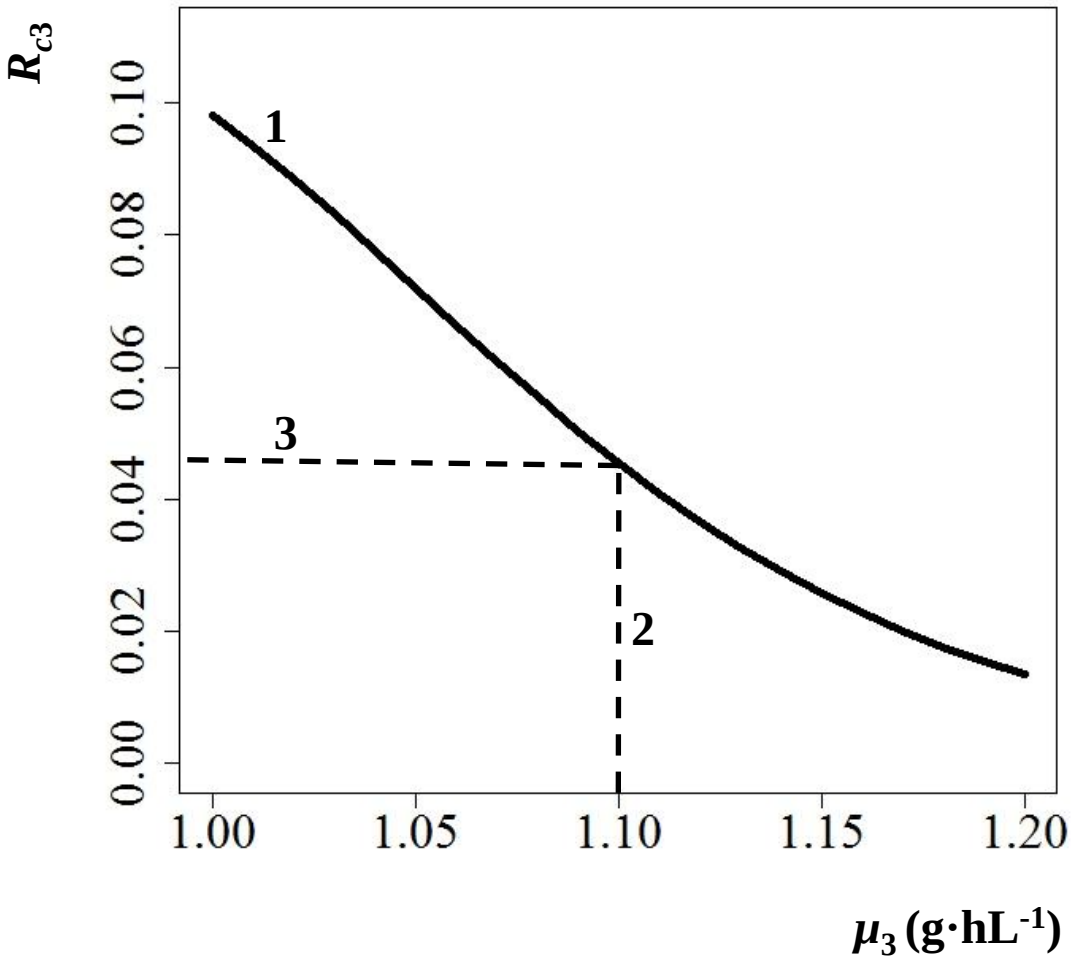
Figure


$C_1 \cap B_1$
$B_1$
$C_1 \cap C_2 \cap B_1$
$C_1 \cap C_2$
$C_1$
$C_2$
$C_2 \cap B_2$
$B_2$
$C_1 \cap C_2 \cap B_2$
$C_1 \cap C_2 \cap B_1 \cap B_2$

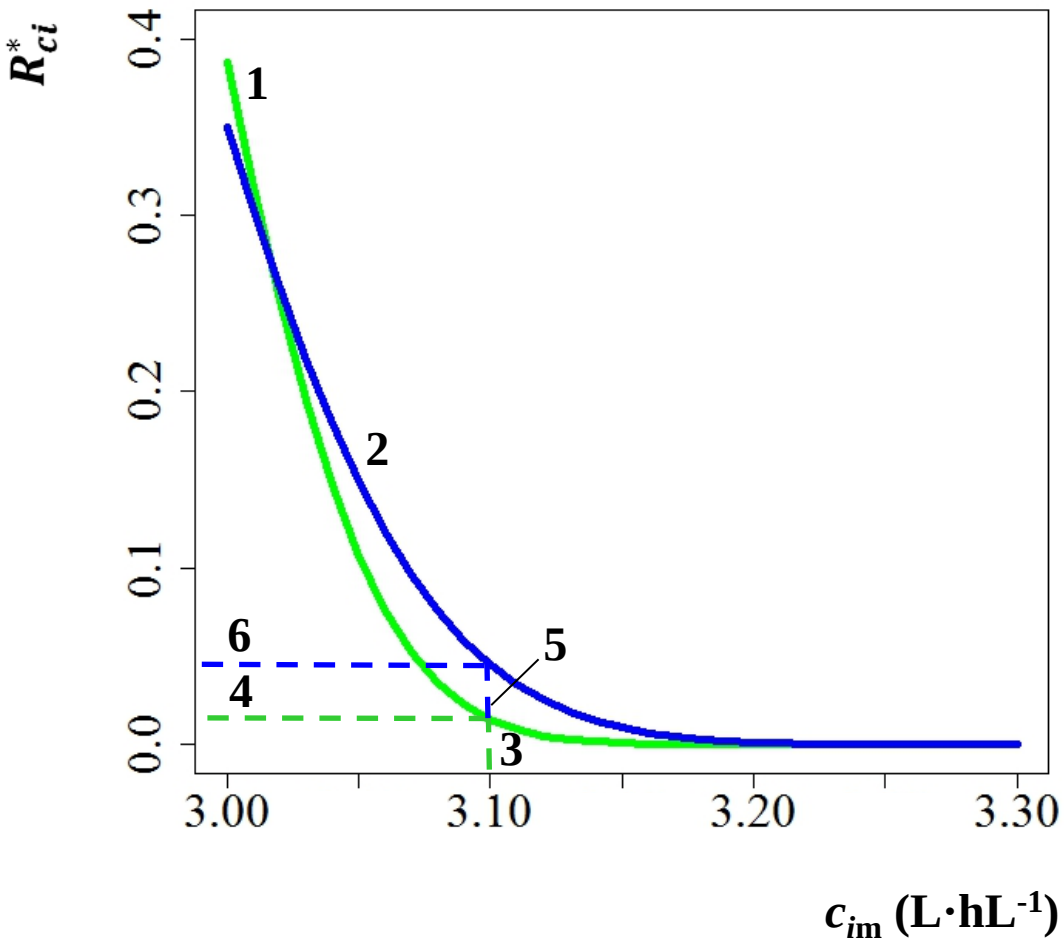
Figure



Figure



Figure



Figure