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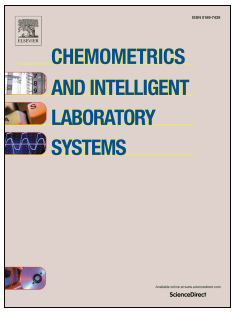
Accepted Manuscript



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PII: S0169-7439(18)30631-2

DOI: https://doi.org/10.1016/j.chemolab.2019.02.010

Reference: CHEMOM 3751

To appear in: *Chemometrics and Intelligent Laboratory Systems*

Received Date: 13 November 2018

Revised Date: 24 February 2019

Accepted Date: 26 February 2019

Please cite this article as: R.J.N. Bettencourt da Silva, F.R. Lourenço, F.R. Pennecchi, D.B. Hibbert, I. Kuselman, Spreadsheet for evaluation of *global* risks in conformity assessment of a multicomponent material or object, *Chemometrics and Intelligent Laboratory Systems* (2019), doi: https://doi.org/10.1016/j.chemolab.2019.02.010.

Spreadsheet for evaluation of global risks in conformity assessment of a multicomponent material or object

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Abstract A user-friendly MS-Excel spreadsheet is developed for evaluation of *global* consumer's and producer's risks in conformity assessment of chemical composition of a multicomponent material or object, when up to four component concentrations are under control. These risks are probabilities of incorrect conformity decisions related to a material batch (lot or similar) randomly drawn from a statistical population of such batches. The probabilities characterize the material quality globally, allowing the prediction of false decisions on conformity of a future batch, based on the future measurement results. The spreadsheet program evaluates risks using Monte Carlo simulations. As input data, the following need to be provided to the software: parameters of normal or lognormal distribution of actual ('true') values of the component concentrations (prior distribution); parameters of the distribution of measurements results at the actual value of the component concentration (likelihood function); and correlation matrices for couples of the actual components' concentrations under control and also for corresponding measurement results. The spreadsheet is validated by comparison of the risk estimates with those calculated in R programing environment by numerical integration of the relevant analytical formulae. The developed Excel file and a demonstration videos of its use are available as electronic supplementary material.

Keywords Conformity assessment · Multicomponent material · Measurement uncertainty · Risk of false decision · Monte Carlo simulations · Spreadsheet

1. Introduction

In our tutorial [1], chemical composition of a multicomponent material or object is considered 'conforming' when the actual ('true') concentration c_i of its i-th component, $i = 1, 2, \ldots, n$, is within the specification, regulation or legal tolerance limits/interval $[T_{Li}, T_{Ui}]$, where T_{Li} and T_{Ui} are the lower and upper limits of the interval, respectively. Comparing the chemical analytical measurement/test result c_{im} of the i-th component concentration with the upper limit T_{Ui}, for example, one has to decide whether the material or object conforms or not. Since a measurement result is represented by a measured value c_{im} and an associated measurement uncertainty [2, 3], two kinds of risk (consumer's and producer's) of a false decision on conformity may arise, each at T_{Li} and T_{Ui}. Continuing the example by considering the upper limit T_{Ui}, the probability of a

false decision that the component concentration does not exceed it, based on the measurement result $c_{im} \leq T_{Ui}$, when the material actually does not conform, i.e. the actual concentration exceeds the upper limit ($c_i > T_{Ui}$), is the 'consumer's risk'. On the other hand, the probability of falsely deciding non-conformity (i.e. $c_{im} > T_{Ui}$, when in fact $c_i \leq T_{Ui}$) is the 'producer's risk'.

For a specified material batch, lot, or an environmental compartment, e.g. ambient air in a certain location at a certain time ('batch' from now on), such risks are referred to as the '*specific* consumer's risk' and the '*specific* producer's risk', respectively. The risks of incorrect conformity assessment of a batch randomly drawn from a statistical population of such batches are the '*global* consumer's risk' $R_{ci(c)}$ and the '*global* producer's risk' $R_{ci(p)}$, respectively, as they characterize the material quality globally. In other words, a *global* risk is the probability of a false decision on conformity of a future batch [4], assuming that conditions of the material production (or composition of the object) will not change.

When conformity assessment for each *i*-th component concentration of a batch of a material is successful (i.e. the particular risks $R_{ci(c)}$ and $R_{ci(p)}$ are small enough), the total probabilities of a false decisions concerning conformity of the material as a whole, (i.e. the total risks $R_{total(c)}$ and $R_{total(p)}$) might still be significant. This is important for correct risk management in a factory producing a medication, an alloy or other multicomponent materials, for environmental monitoring and similar tasks. Modeling and evaluating the total risks in conformity assessment of a multicomponent material or object due to measurement uncertainties are developed by us using a Bayesian approach and R programing [5-8]. In particular, core of the R codes for calculation of the risks for uncorrelated and correlated data are published in papers [6] and [8], respectively. A user-friendly spreadsheet program for evaluating *specific* risks of false decisions in conformity assessment of a multicomponent material or object was presented in the tutorial [1] to make calculations more accessible than in the R programming environment.

In the present paper, a new spreadsheet MS Excel program is described for calculation of *global* risks. This program, as the program for evaluating *specific* risks [1], is also accessible for use in quality control, measurement and testing (chemical analytical) laboratories, and does not require special skill in programming by laboratory staff. The spreadsheet is validated by comparison of the results with those obtained in the R programming environment by numerical integration of the relevant analytical formulae, using published examples on denatured alcohols [5], total suspended particle matters in ambient air [6], a medication [7], and an alloy [8]. The

validated spreadsheet for calculation of *global* risks and a demonstration videos of its use are available as electronic supplementary material.

2. Calculation of *global* risks

To decrease the risks, besides the tolerance limits for actual concentration values c_i, acceptance limits for measurement results $c_{i\mathrm{m}}$ (e.g. internal factory limits) can be applied taking into account the measurement uncertainty [3, 4]. However, if the measurement uncertainty is already considered when setting tolerance limits, they coincide with the acceptance limits, as assumed in the spreadsheet. In such cases, the *i*-th particular *global* risk is calculated as the following double integral:

$$R_{ci} = \iint f(c_i) f(c_{i\mathrm{m}}|c_i)\mathrm{d}c_{i\mathrm{m}}\mathrm{d}c_i, \qquad (1)$$

where $f(c_i)$ is the pdf of the distribution of c_i values (the prior pdf), $f(c_{i\mathrm{m}}|c_i)$ is the pdf of the distribution of measurement results $c_{i\mathrm{m}}$ at the actual value c_i (characterizing the likelihood function). The limits of integration depend on the type of the risk: consumer's or producer's [4, 9]. For example, for calculation of the consumer's risk, when c_i is required to be smaller than $T_{\mathrm{U}i}$, the limits of the outer integral (relevant to c_i) are from $T_{\mathrm{U}i}$ to ∞, whereas the limits of the inner integral (relevant to $c_{i\mathrm{m}}$) are from 0 to $T_{\mathrm{U}i}$.

Note, the product of $f(c_i)$ and $f(c_{i\mathrm{m}}|c_i)$ is a joint pdf $f(c_{i\mathrm{m}}, c_i)$ of actual values and measurement results. The total *global* risk is, consequently, a more complicated integral of the multivariate joint pdf of actual values and measurement results of the concentrations of the *n* components under control in a batch [5-8].

2.1. Simulations

In order to estimate the *global* risk by MC method, simulations are necessary for 1) actual *i*-th component concentration $c_{il}(\mathrm{s})$ in the *l*-th material batch, which might be produced, l = 1, 2, …, N; and 2) future measurement result $c_{il\mathrm{m}}(\mathrm{s})$ of the *i*-th component concentration in the *l*-th batch.

An actual component concentration $c_{il}(\mathrm{s})$ is simulated as drawn from the population of the material batches, according to the prior pdf. For each simulated $c_{il}(\mathrm{s})$, a corresponding measurement result $c_{il\mathrm{m}}(\mathrm{s})$ could be simulated by drawing it from the pdf characterizing the

likelihood function at this $c_{il}(\mathrm{s})$ value. In practice, $c_{il\mathrm{m}}(\mathrm{s})$ is obtained by summing the simulated actual concentration $c_{il}(\mathrm{s})$ and a simulated measurement error $e_{il}(\mathrm{s})$ drawn from a pdf equal to that characterizing the likelihood function, but shifted to zero. Note, the standard deviation of such pdf, at the same actual value of the concentration, is equal to the standard measurement uncertainty u_i of the *i*-th component concentration. Thus,

$$c_{il\mathrm{m}}(\mathrm{s}) = c_{il}(\mathrm{s}) + e_{il}(\mathrm{s}). \quad (2)$$

When the likelihood function is described by a normal pdf, simulated measurement errors $e_{il}(\mathrm{s})$ are drawn from N(0, u_i). They are distributed symmetrically around zero and so can be positive and negative. If the actual component concentration value c_i is close to zero, e.g. for an impurity, the *l*-th simulated value $c_{il}(\mathrm{s})$ is also small and even negative in some cases. Therefore, $c_{il\mathrm{m}}(\mathrm{s})$ also might be negative. Since any concentration is a non-negative quantity by definition, simulated negative $c_{il}(\mathrm{s})$ and $c_{il\mathrm{m}}(\mathrm{s})$ are removed and corresponding simulations are not counted in the total number of simulations *N*. This operation is equivalent to using in formula (1) truncated normal distributions in the interval [0, ∞] for both actual values c_i and measurement results $c_{i\mathrm{m}}$.

The simulations of actual concentrations $c_{il}(\mathrm{s})$ and measurement errors $e_{il}(\mathrm{s})$ are performed by the MC method using a generator of correlated normally distributed variables, based on the Cholesky decomposition [10] of the covariance matrix of the involved variables (the actual values and the measurement results). Note, any covariance matrix by definition is positive definite, as required for the Cholesky factorization. The input data are mean μ (location) and standard deviation σ (scale value) of actual concentration values, the standard measurement uncertainty (scale value of the normally-distributed errors), as well as the correlation coefficients r_{ij} between *i*-th and *j*-th actual values and *i*-th and *j*-th measurement results, $i \neq j$. Output data are the simulated values. The random values generator works for independent as well as for correlated normally-distributed variables. It can also generate independent log-transformed actual values of the component concentrations, characterised by the mean and standard deviation of the transformed variable. The simulated values of the lognormally distributed concentrations are hence obtained as the exponents of the simulated log-transformed concentrations. In this case, simulation of correlated variables is not possible.

Thus, the simulations can be used for uncorrelated normal or lognormal priors and normal likelihoods, i.e. when zero correlation coefficients ($r_{ij} = 0$) are entered. When both priors and likelihoods are normal, any r_{ij} between –1 and 1 can be entered. Different correlation matrices for the normal prior and likelihood, and absolute or relative standard measurement uncertainty (u_i or u_{reli}, respectively) for each *i*-th component are allowed.

2.2. Spreadsheet

The particular *global* consumer's risk $R_{ci(\mathrm{c})}$ is evaluated as the number of simulated measurement results of the *i*-th component concentrations $c_{il\mathrm{m}}(\mathrm{s})$ within the tolerance interval, when corresponding actual concentration values $c_{il}(\mathrm{s})$ are outside this interval ("False IN"), divided by the number of simulations *N*. The *global* particular producer's risk $R_{ci(\mathrm{p})}$ is evaluated as the number of the $c_{il\mathrm{m}}(\mathrm{s})$ outside the tolerance interval, when corresponding $c_{il}(\mathrm{s})$ are within this interval ("False OUT"), divided by *N*. The spreadsheet "Global4Risk_Macros_to_be_Activated.xlsm", attached as electronic supplementary material, performs *N* up to 50000 simulations of actual values and measurement results of concentrations of each component.

The sheet "Particular_Risk" in the file "Global4Risk_Macros_to_be_Activated.xlsm" is a graphical representation of simulated measurement results and corresponding actual component concentration values used for evaluation of particular *global* risks. There are measurement results correctly situated together with corresponding actual values within the tolerance interval (legend "IN"), correctly situated outside the tolerance interval (legend "OUT"), as well as incorrectly situated within ("False IN") and out ("False OUT") the tolerance interval. Fig. 1 shows an example of such graphical representation.

Fig. 1

The sheet "Univariate_Graph" combines in the same figure the normalised frequencies of the simulated actual values and measurement results of concentrations of the *i*-th component (not reproduced here).

The total *global* consumer's risk $R_{\mathrm{total(c)}}$ is evaluated as the number of cases when simulated measurement results for all components $i = 1, 2, \ldots. n$ are within their tolerance intervals, but at least one of the *n* simulated actual concentration values is outside its interval ("False IN"), divided by the total number of cases *N*. The total *global* producer's risk $R_{\mathrm{total(p)}}$ is the number of cases when at least one simulated measurement result is outside its tolerance interval, while all

simulated actual concentration values are within their intervals ("False OUT"), divided by the total number of simulations *N*.

The sheet "Total Risk" is the graphical representation of simulated measurement results of concentrations of two of the *n* components, where the "False IN" and "False OUT" cases for any *i*-th of the *n* components are identified. The points "IN" (correctly conforming) are overlapped by all points. The points "OUT" (correctly nonconforming) are overlapped by all other points excepting "IN". The points "False IN" overlap all points excepting "False OUT", which also overlap all other points. The cells K10, K12 and M12 of the sheet "Input Data" allows selecting the variables represented on such plots.

Fig. 2

Fig. 2 shows an example of the graphical representation of simulated measurement results for evaluation of the total *global* risks when two components are under control, i.e. $n = 2$.

Fig. 3

Fig. 3 is related to the same two components, as in Fig. 2, but in this case a third component is considered in addition. The third component is responsible for an increase of "False OUT" cases and corresponding increase of the total *global* producer's risk. The total g*lobal* consumer's risk is also increased but this is invisible in the plot, as the "False IN" points are overlapped by "False OUT" points.

When simulated $c_{il\mathrm{m}}$ and c_{il} values are positive definite (e.g. for concentrations of main components of a material) negative realizations are practically impossible and the calculation option "No constraints" at line 43 is suitable. However, a choice of the respective option "No constraints" or "Cancel negative values" at line 43 should be carefully made, since the option "No constrains" might lead to incorrect results when the distance of the concentration values from zero is small taking into account the measurement uncertainty. The sheet "Particular_Risk" providing graphical representations of simulated measurement results vs. actual values (as in Fig. 1) can be helpful for control of the right choice of "No constraints". If negative values are indicated, the calculations should be repeated with the option "Cancel negative values".

The developed spreadsheet installed on a regular personal computer can perform a run consisting of $N = 50000$ simulations according to formula (2) and calculations of the risks in just few seconds. The repetition of 30 runs takes less than two minutes. To start calculations with the spreadsheet, the macros should be activated as explained in the video "Macros_Activation.mp4". Then, input of raw data and further calculation steps are explained in the video

"Global4Risk.xlsm: Demo_Global4Risk.xlsm.mp4". Both the videos are available as electronic supplementary material.

3. Validation of the spreadsheet

3.1. Validation criteria

ISO 9000 [11] defines validation as "a confirmation, through the provision of objective evidence, that the requirements for a specific intended use or application have been fulfilled". Similar definitions are in JCGM 200 [12] and other documents compared in the Eurachem Guide [13]. There are strict requirements in the field of software for medical devices [14, 15]. Validation of a computer program in testing and calibration laboratories is required by ISO/IEC 17025 [16] and FDA Guidelines [17]. Anyway, the extent of validation is always a balance between costs, risks and technical possibilities [13, 18, 19].

The formulas and macros in the spreadsheet are protected from overwriting or change without password [20]. However, the *global* risk estimates produced by the developed program are affected by the variability of the combination of randomly generated information. This variability decreases with increasing number of simulations *N*. Therefore, the following two validation criteria were set on the current stage of the program development: 1) a mean risk value $\bar{R}$ obtained from 30 MC runs, each of N = 50000 simulations, should not differ statistically from the value calculated by numerical integration of the relevant analytical formulae, performed in the R programming environment [5-8]; and 2) the standard deviation s_R of the mean risk value $\bar{R}$ is to be not greater than 10 % of $\bar{R}$.

The validation is performed by comparison of the spreadsheet results with the risk values published in ref. [5-8]. A total of 7 scenarios of the total *global* (consumer's and producer's) risk evaluation were used for this comparison.

3.2. Results of the validation

The estimates of risk are presented in Tables 1-4. The examples of *global* risks calculated for scenarios with the independent (hence, uncorrelated) variables are in Tables 1 and 2. Scenario #1 in Table 1 relates to concentrations of two denaturants under customs control in a denatured alcohol, while scenario #2 - to concentrations of three denaturants [5]. In these scenarios the

consumer is the custom, and the producer is the importer of the alcohol. Data in Table 2 describe a case of ambient air contaminated by total suspended particle matters generated in three stone quarries, and the *global* risks of inhabitants of the industrial zone (the consumer). The producer in this case is the quarry owner [6]. Table 3 contains scenario #1, when measurement results of concentrations of four active components in a medication are uncorrelated, and scenario #2 – when correlation among the measurement results is strong. The consumer is a sick person taking a medication, while the producer is the pharmaceutical company [7]. Similar scenarios are in Table 4, related to the control of concentrations of rhodium and sum of eight impurities in a PtRh alloy [8]. Correlation of the measurement results of these two alloy components, not taken into account in scenario #1, is statistically significant but weak in scenario #2. The consumer is a purchaser of the alloy, and the producer is the owner of the factory producing this alloy.

The mean risk values $\bar{R}$ and their standard deviation s_R, obtained from 30 MC runs, each made with N = 50000 simulations, are shown in the tables. Standard deviations s_R are rounded up to one or two significant figures, and $\bar{R}$ values are expressed with the same number of decimal places.

The validation of the MS-Excel spreadsheet is satisfactory, since 1) the difference between the analytical results of the risk evaluation in the R environment and the spreadsheet estimates do not exceed the confidence interval $\bar{R} \pm ts_R$, where t is a quantile of Student-t distribution, e.g. equal 2.8 at the 99 % level of confidence and 28 degrees of freedom; and 2) the s_R values as a rule are not greater than 3-5 % of corresponding mean risk values, and do not exceed 10 % of $\bar{R}$.

4. Conclusions

The developed MS-Excel spreadsheet is a user-friendly program for evaluation of *global* risks (probabilities) of false decisions in conformity assessment of chemical composition of a multicomponent material or object, when up to four component concentrations are under control. Calculations with this program allow characterization of the conformity of a batch, lot or similar unit of a material or object, which might be produced with the same conditions as previous ones.

The spreadsheet has been successfully validated by comparison of obtained risk estimates with those calculated in the R programing environment by numerical integration of the relevant analytical formulae. The MS-Excel file and a videos explaining the spreadsheet use are available as electronic supplementary material.

The developed program complements earlier published spreadsheets for calculation of *specific* risks and also will be helpful in different conformity assessment tasks related to multicomponent materials or objects.

Electronic supplementary material

- File to process the *global* risk calculation: Global4Risk_Macros_to_be_Activated.xlsm

- Video explaining activation of the macros: Macros_Activation.mp4

- Video explaining the use of the file Global4Risk.xlsm: Demo_Global4Risk.xlsm.mp4

Acknowledgment

This research was supported in part by the International Union of Pure and Applied Chemistry (IUPAC Projects 2016-007-1-500 and 2018-004-1-500).

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Figure captions

Fig. 1. Graphical representation of simulated actual concentration values $c_{1l}(\mathbf{s})$ of component 1 and corresponding measurement results $c_{1lm}(\mathbf{s})$ used for evaluation of a particular *global* risk. The limit of the tolerance interval is shown by dotted black lines. The measurement results correctly situated within the tolerance interval ("IN") are indicated by dark blue points in the upper right quarter of the plot, while the results correctly situated outside the tolerance interval ("OUT") - by dark red points in the lower left quarter of the plot. The measurement results incorrectly situated within the tolerance interval ("False IN") are shown by Cambridge blue points in the upper left quarter of the plot, while the results incorrectly situated outside the tolerance interval ("False OUT") – by the light-red points in the lower right quarter of the plot.

Fig. 2. Graphical representation of simulated measurement results $c_{il\mathrm{m}}(\mathbf{s})$ of concentrations of two components (*i* = 1 and 2) used for evaluation of the total *global* risks. The points and their colours used are as explained in Fig. 1 caption.

Fig. 3. Graphical representation of simulated measurement results $c_{il\mathrm{m}}(\mathbf{s})$ of concentrations of two (*i* = 1 and 2) of the three components under control used for evaluation of the total *global* risks. The points and their colours used are as explained in Fig. 1 caption. The third component is responsible here for a larger number of false decisions in comparison with those shown in Fig. 2.

Table 1. Risks of false decision in conformity assessment of denatured alcohols with two or three denaturants [5]

#	*i*	Actual concentration/prior	Measurement uncertainty	Limit	Analytical risk estimate (%)				MS-Excel risk estimate (%)			
					$R_{ci(\mathrm{c})}$	$R_{ci(\mathrm{p})}$	$R_{\mathrm{total(c)}}$	$R_{\mathrm{total(p)}}$	$\bar{R}_{ci(\mathrm{c})}; s_R$	$\bar{R}_{ci(\mathrm{p})}; s_R$	$\bar{R}_{\mathrm{total(c)}}; s_R$	$\bar{R}_{\mathrm{total(p)}}; s_R$
1	1	μ_1 = 3.15; σ_1 = 0.1575 (N&I)	u_1 = 0.05	$T_{\mathrm{L1}} = 3$	2.7	3.8			2.6; 0.1	3.8; 0.1		
	2	μ_2 = 3.15; σ_2 = 0.1575 (N&I)	u_2 = 0.07	$T_{\mathrm{L2}} = 3$	3.4	5.6	4.8	7.6	3.4; 0.1	5.5; 0.1	4.8; 0.1	7.5; 0.1
2	1	μ_1 = 3.15; σ_1 = 0.1575 (N&I)	u_1 = 0.05	$T_{\mathrm{L1}} = 3$	2.7	3.8			2.6; 0.1	3.8; 0.1		
	2	μ_2 = 3.15; σ_2 = 0.1575 (N&I)	u_2 = 0.07	$T_{\mathrm{L2}} = 3$	3.4	5.6	6.6	11.4	3.4; 0.1	5.5; 0.1	6.5; 0.1	11.3; 0.1
	3	μ_3 = 1.10; σ_3 = 0.11 (N&I)	u_3 = 0.07	$T_{\mathrm{L3}} = 1$	4.6	8.5			4.5; 0.1	8.5; 0.1		

- scenario number; *i* - component number; N&I - normally distributed and independent; $T_{\mathrm{L}i}$ - lower limit; $\bar{R}$ - mean value; s_R - standard deviation.

Table 2. Risks of false decisions in conformity assessment of total suspended particulate matter concentration in ambient air near three stone quarries [6]

#	i	Actual concentration/prior	Measurement uncertainty	Limit	Analytical risk estimate (%)				MS-Excel risk estimate (%)			
					$R_{ci(\mathrm{c})}$	$R_{ci(\mathrm{p})}$	$R_{\mathrm{total(c)}}$	$R_{\mathrm{total(p)}}$	$\bar{R}_{ci(\mathrm{c})}; s_R$	$\bar{R}_{ci(\mathrm{p})}; s_R$	$\bar{R}_{\mathrm{total(c)}}; s_R$	$\bar{R}_{\mathrm{total(p)}}; s_R$
I	1	μ_1 = -2.326; σ_1 = 0.434 (LN&I)	u_{rel1} = 0.07	$T_{\mathrm{U1}} = 0.2$	0.58	0.74			0.58; 0.03	0.73; 0.03		
	2	μ_2 = -2.031; σ_2 = 0.280 (LN&I)	u_{rel2} = 0.07	$T_{\mathrm{U2}} = 0.2$	1.04	1.52	1.9	2.6	1.06; 0.05	1.54; 0.06	1.9; 0.1	2.6; 0.1
	3	μ_3 = -2.338; σ_3 = 0.403 (LN&I)	u_{rel3} = 0.07	$T_{\mathrm{U3}} = 0.2$	0.46	0.62			0.46; 0.03	0.61; 0.03		

- scenario number; i - quarry number; LN&I - lognormally distributed and independent; $T_{\mathrm{U}i}$ - upper limit; $\bar{R}$ - mean value; s_R- standard deviation.

Table 3. Risks of false decisions in conformity assessment of a medication with four active components under control and correlated test results [7]

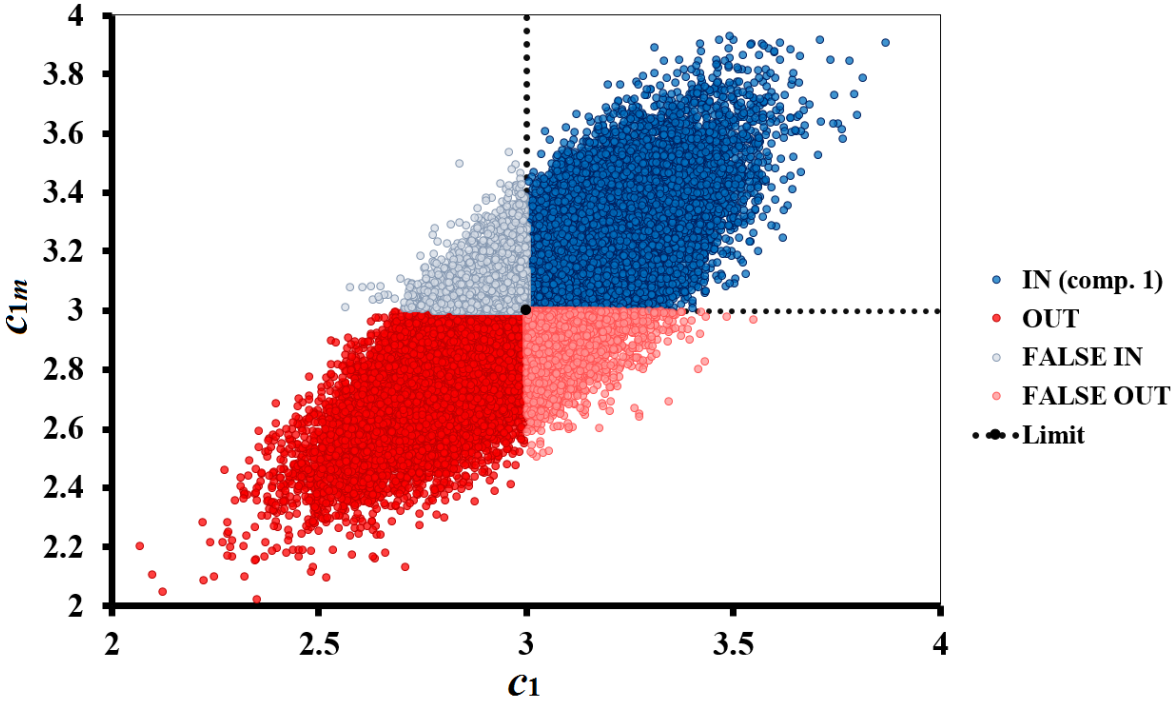
#	i	Actual concentration/prior	Measurement uncertainty	Limits $[T_{Li}, T_{Ui}]$	Analytical risk estimate (%)				MS-Excel risk estimate (%)			
					$R_{ci(c)}$	$R_{ci(p)}$	$R_{total(c)}$	$R_{total(p)}$	$\bar{R}_{ci(c)}; s_R$	$\bar{R}_{ci(p)}; s_R$	$\bar{R}_{total(c)}; s_R$	$\bar{R}_{total(p)}; s_R$
1	1	μ_1 = 99.18; σ_1 = 1.37 (N&I)	u_{rel1} = 0.028	[95, 105]	0.05	11.8			0.05; 0.01	11.8; 0.2		
	2	μ_2 = 97.7; σ_2 = 1.02 (N&I)	u_{rel2} = 0.028	[95, 105]	0.18	18.2			0.19; 0.02	18.2; 0.2		
	3	μ_3 = 99.33; σ_3 = 1.05 (N&I)	u_{rel3} = 0.028	[95, 105]	0.001	10.1	0.19	45	0.001; 0.001	10.1; 0.1	0.18; 0.02	43; 1
	4	μ_3 = 98.94; σ_3 = 1.22 (N&I)	u_{rel4} = 0.028	[95, 105]	0.03	11.9			0.03; 0.01	11.9; 0.2		
2	1	μ_1 = 99.18; σ_1 = 1.37 (N&C)	u_{rel1} = 0.028	[95, 105]	0.05	11.8			0.05; 0.01	11.8; 0.2		
	2	μ_2 = 97.7; σ_2 = 1.02 (N&C)	u_{rel2} = 0.028	[95, 105]	0.18	18.2			0.19; 0.02	18.2; 0.2		
	3	μ_3 = 99.33; σ_3 = 1.05 (N&C)	u_{rel3} = 0.028	[95, 105]	0.001	10.1	0.16	30	0.001; 0.001	10.1; 0.1	0.19; 0.02	30; 1
	4	μ_4 = 98.94; σ_4 = 1.22 (N&C)	u_{rel4} = 0.028	[95, 105]	0.03	11.9			0.03; 0.01	11.9; 0.2		

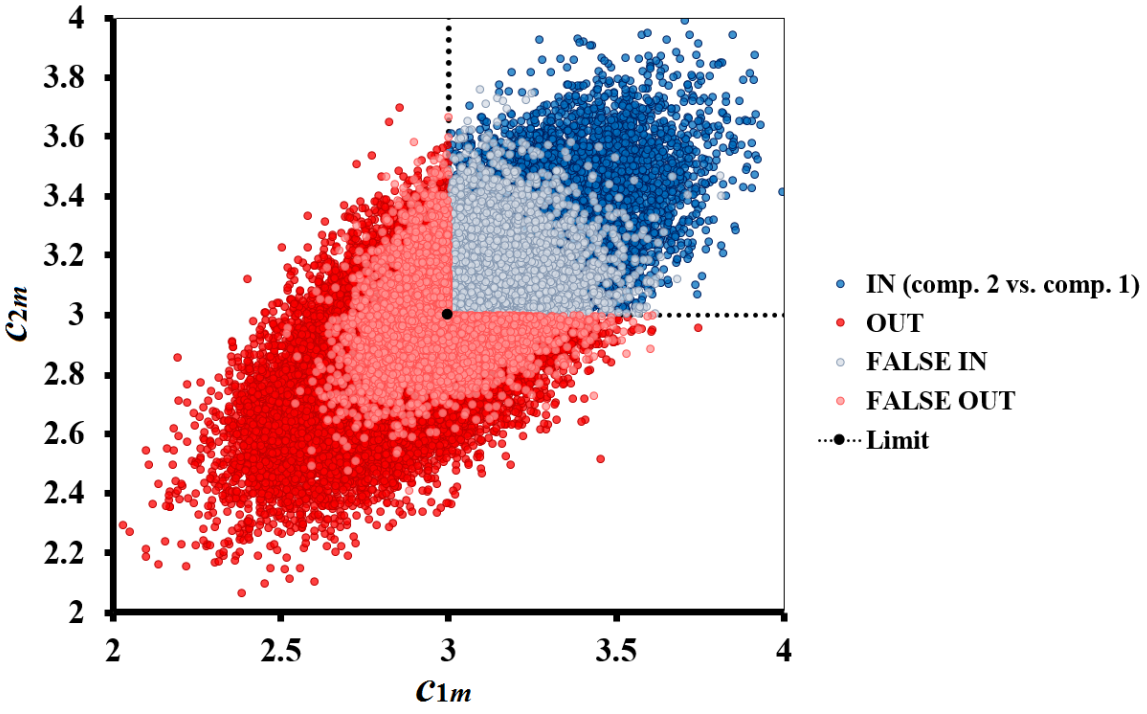
- scenario number; i - component number; N&I - normally distributed and independent; N&C - normally distributed and correlated with the other components concentrations when the Pearson's correlation coefficients r_{ij} = 0.7; T_{Li} - lower limit; T_{Ui} - upper limit; $\bar{R}$ - mean value; s_R - standard deviation.

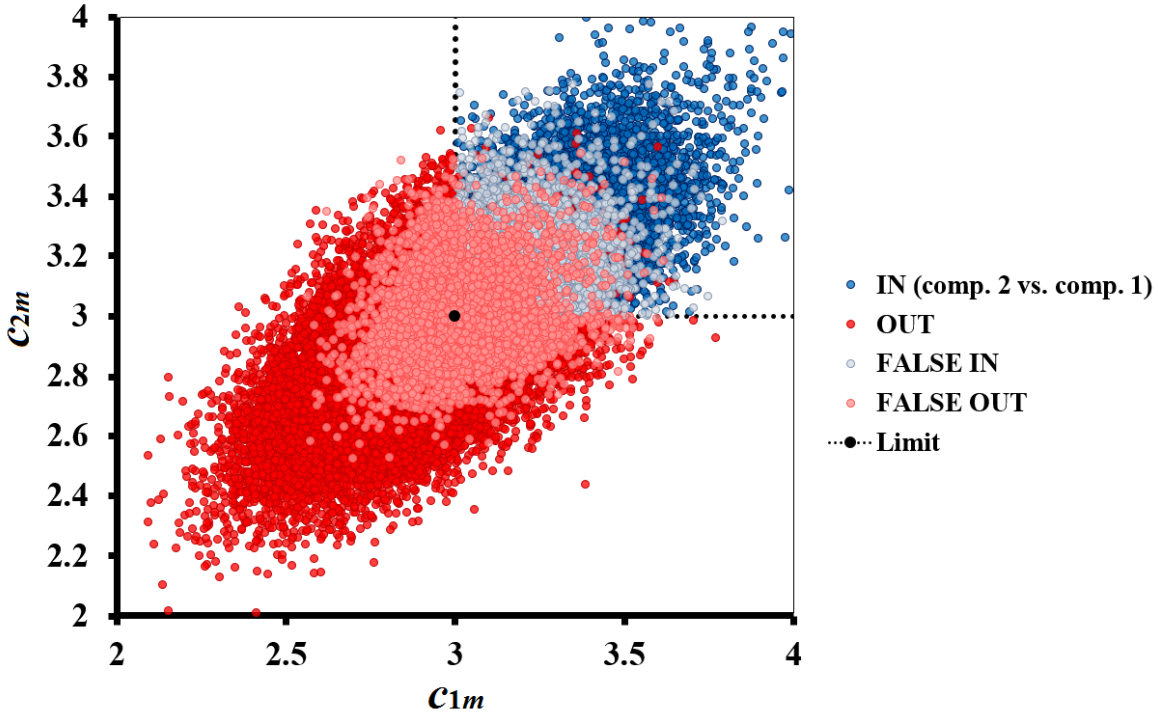
Table 4. Risks of false decisions in conformity assessment of a PtRh alloy with four components under control and correlated test results [8]

#	i	Actual concentration/prior	Measurement uncertainty	Limits $[T_{Li}, T_{Ui}]$	Analytical risk estimate (%)				MS-Excel risk estimate (%)			
					$R_{ci(c)}$	$R_{ci(p)}$	$R_{total(c)}$	$R_{total(p)}$	$\bar{R}_{ci(c)}; s_R$	$\bar{R}_{ci(p)}; s_R$	$\bar{R}_{total(c)}; s_R$	$\bar{R}_{total(p)}; s_R$
1	1	μ_1 = 7.457; σ_1 = 0.073 (N&I)	u_1 = 0.04	[7.3, 7.7]	0.47	2.0			0.47; 0.02	2.0; 0.1		
	2	μ_2 = 0.059; σ_2 = 0.021 (N&I)	u_{rel2} = 0.18	[0, 0.18]	3.7e-05	1.3e-05	0.47	2.0	< 0.002	0.004; 0.002	0.47; 0.03	2.0; 0.1
2	1	μ_1 = 7.457; σ_1 = 0.073 (N&C)	u_1 = 0.04	[7.3, 7.7]	0.47	2.0			0.47; 0.02	2.0; 0.1		
	2	μ_2 = 0.059; σ_2 = 0.021 (N&C)	u_{rel2} = 0.18	[0, 0.18]	3.7e-05	1.3e-05	0.51	2.1	< 0.002	0.004; 0.002	0.48; 0.03	2.0; 0.1

- scenario number; i - component number; N&I - normally distributed and independent; N&C - normally distributed and correlated when the Pearson's correlation coefficients r_{ij} = 0.228; T_{Li} - lower limit; T_{Ui} - upper limit; $\bar{R}$ - mean value; s_R - standard deviation.







HIGHLIGHTS

- A new spreadsheet program for evaluating global risks of false decisions in conformity assessment is developed.
- The program algorithm is based on the Monte Carlo simulations.
- The program was validated by comparison of the risk estimates with the results calculated in R programming environment.
- The spreadsheet and audio-video instructions explaining the program use are provided as electronic supplements.