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Francesca R. Pennecchi, Ilya Kuselman, Ricardo J.N.B. da Silva, D. Brynn Hibbert



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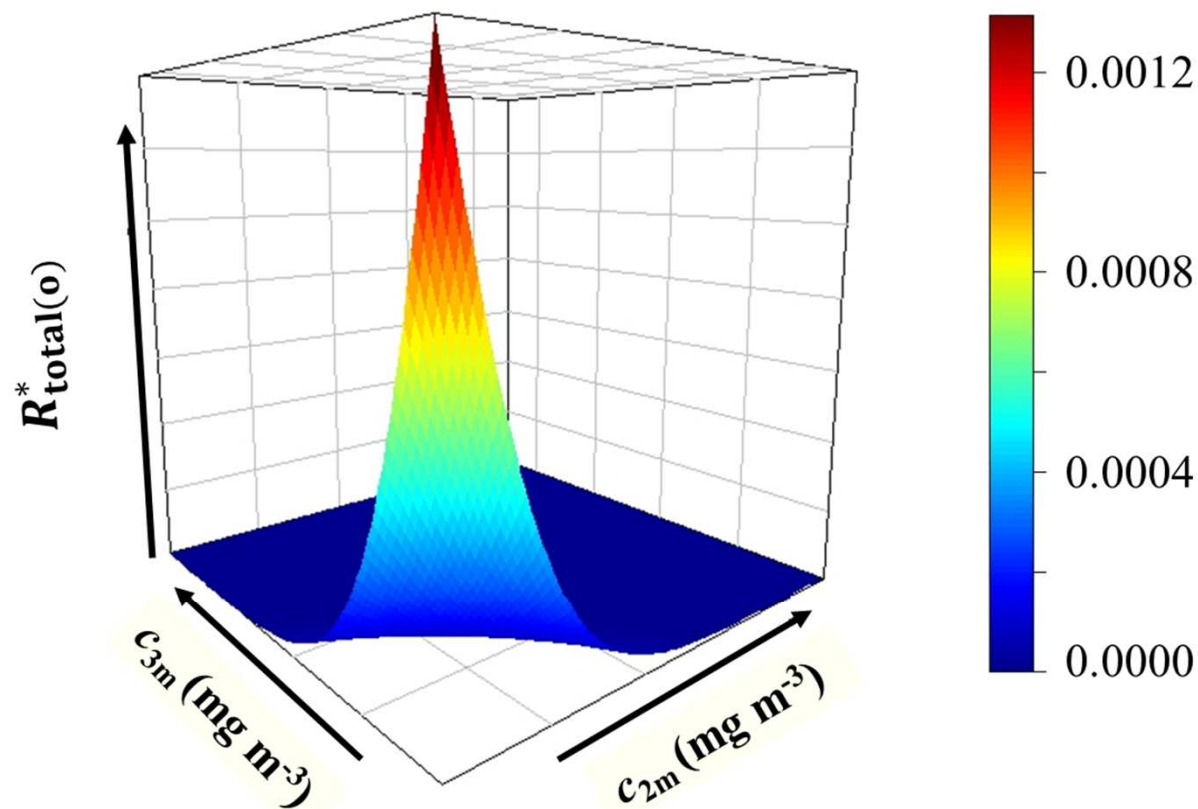
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Dependence of the total risk of overestimation  $R_{total(o)}^*$  of suspended particulate matter concentration in ambient air on the measurement results  $c_{im}$  in proximity to the three quarries ( $c_{1m} = 0.250 \text{ mg m}^{-3}$ ;  $c_{2m}$  and  $c_{3m}$  are varying from  $0.210$  to  $0.300 \text{ mg m}^{-3}$ ).

**Risk of a false decision on conformity of an environmental  
compartment due to measurement uncertainty of concentrations of  
two or more pollutants**

**Francesca R. Pennechi<sup>a</sup>, Ilya Kuselman<sup>b,\*</sup>, Ricardo J. N. B. da Silva<sup>c</sup>, D. Brynn Hibbert<sup>d</sup>**

<sup>a</sup> *Istituto Nazionale di Ricerca Metrologica (INRIM), Strada delle Cacce 91, 10135 Turin, Italy*

<sup>b</sup> *Independent Consultant on Metrology, 4/6 Yarehim St., 7176419 Modiin, Israel*

<sup>c</sup> *Centro de Química Estrutural, Faculdade de Ciências da Universidade de Lisboa, Edifício C8,  
Campo Grande, 1749-016 Lisboa, Portugal*

<sup>d</sup> *School of Chemistry, UNSW Sydney, Sydney NSW 2052, Australia*

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

E-mail address: [ilya.kuselman@bezeqint.net](mailto:ilya.kuselman@bezeqint.net) (I. Kuselman)

4/6 Yarehim St., Modiin, 7176419 Israel

## 1. Introduction

Actual ('true') concentration  $c_i$  of the  $i$ -th pollutant,  $i = 1, 2, \dots, n$ , in an environmental compartment, e.g. ambient air (Duursma and Carroll (1996); TIMBRE project, Online), should not exceed a regulation or legal tolerance upper limit  $T_{Ui}$ . 'Concentration' is used here as a generic term (Cvitaš, 1996; Tolhurst, 2005; Fuentes-Arderiu, 2013). Comparing a chemical analytical test/measurement result  $c_{im}$  of the  $i$ -th pollutant concentration with the  $T_{Ui}$  value, one should decide whether the compartment conforms to the regulation or not. Since any result  $c_{im}$  has an associated measurement uncertainty (Ellison and Williams, 2012; Magnusson et al., 2012), several kinds of risk of a false decision on conformity of the compartment may arise.

The probability of a decision that the actual pollutant concentration does not exceed the limit since  $c_{im} \leq T_{Ui}$ , when it is not correct (i.e.  $c_i > T_{Ui}$ ), is named 'consumer's risk'. The 'consumer' in the present paper is a habitant whose quality of life (including health) depends on adequate control of the pollutant. Thus, the consumer's risk is the probability of underestimation of  $c_i$  due to measurement uncertainty associated with  $c_{im}$ .

On the other hand, the probability of falsely rejecting the decision on conformity of the compartment to the regulation (i.e.  $c_{im} > T_{Ui}$  when  $c_i \leq T_{Ui}$ ) is the 'producer's risk'. The 'producer' here is a plant or another organization – a source of the environment pollution, obliged to pay a fine and/or to invest money for an unnecessary reduction of the pollutant concentration in the case of false nonconformity. The producer's risk is therefore the probability of overestimation of  $c_i$  due to measurement uncertainty in  $c_{im}$ .

For a specified compartment, e.g. ambient air in a certain location at a certain time, such risks are referred to as the 'specific consumer's risk' of underestimation  $R_{ci(u)}^*$  and the 'specific

producer's risk' of overestimation  $R_{ci(o)}^*$  for  $i$ -th particular pollutant concentration. The risks of incorrect conformity assessment of a compartment randomly drawn from a statistical population of such compartments are the 'global consumer's risk' of underestimation  $R_{ci(u)}$  and the 'global producer's risk' of overestimation  $R_{ci(o)}$ , respectively, as they characterize the environmental quality globally. Evaluation of the particular risks (both specific and global) is described in the JCGM 106 (2012) based on a Bayesian approach to conformity assessment.

However, when concentrations of two or more pollutants are controlled, pollutant-by-pollutant evaluation of the risks is not complete in general, as it does not give an answer to the question of the probability of a false decision on the overall compartment conformity. If conformity assessment for each  $i$ -th pollutant concentration of a compartment is successful, i.e. the particular specific  $R_{ci}^*$  or global  $R_{ci}$  risks of both under- and overestimation are small enough, the total probability of a false decision concerning conformity of the compartment as a whole (the *total* specific  $R_{total}^*$  or *total* global  $R_{total}$  risk) might still be significant.

A scheme summarizing the used terminology is shown in Fig. 1, where the particular risks described in the JCGM 106 (2012) are shown at the top of the scheme. The *total risk evaluation*, as the task of the IUPAC Project (2016), is highlighted by an ellipse at the bottom of the scheme.

Using the law of total probability for the case of independent quantities (pollutant concentration values and corresponding measurement results) the total risk of underestimation can be evaluated as a combination of the particular risks (Kuselman et al., 2017a). For example, for three pollutions  $i = 1, 2, 3$ , assuming independent actual values of each pollutant concentration  $c_i$  and independent corresponding measurement results  $c_{im}$ , the total specific risk of underestimation is:

$$\begin{aligned}
 R_{\text{total}(u)}^* &= R_{c1(u)}^* + R_{c2(u)}^* + R_{c3(u)}^* - R_{c1(u)}^* R_{c2(u)}^* - R_{c1(u)}^* R_{c3(u)}^* - R_{c2(u)}^* R_{c3(u)}^* + \\
 &R_{c1(u)}^* R_{c2(u)}^* R_{c3(u)}^*.
 \end{aligned} \tag{1}$$

E.g., for all the particular specific risks  $R_{ci(u)}^* = 0.05$ , the total specific risk by formula (1) is  $R_{\text{total}}^* = 0.14$ . Total global risk of underestimation for the three pollutants is:

$$\begin{aligned}
 R_{\text{total}(u)} &= \\
 &P(C_2)P(C_3)R_{c1(u)} + P(C_1)P(C_3)R_{c2(u)} + P(C_1)P(C_2)R_{c3(u)} - P(C_3)R_{c1(u)}R_{c2(u)} - \\
 &P(C_2)R_{c1(u)}R_{c3(u)} - P(C_1)R_{c2(u)}R_{c3(u)} + R_{c1(u)}R_{c2(u)}R_{c3(u)},
 \end{aligned} \tag{2}$$

where  $P(C_i)$  is the probability that a measurement result  $c_{im}$  is acceptable, i.e.  $c_{im} \leq T_{Ui}$ . For example, for the particular risks  $R_{ci} = 0.05$  and probabilities  $P(C_i) = 0.90$  for all  $i$ , formula (2) gives  $R_{\text{total}} = 0.12$ .

General expressions for evaluating the total risk of underestimation for any number  $n$  of the material components (or pollutants of an environmental compartment) are also provided in the mentioned above reference. Treatment of correlated measurement results for total risk evaluation is discussed in the paper by Kuselman et al. (2017b).

In the present paper, the total risk of overestimation (producer's risk) is formulated in the same Bayesian framework for uncorrelated test results as it was applied in the previous work (Kuselman et al., 2017a) for underestimation (consumer's risk). Core code developed in R programming environment (the R project, Online) for corresponding calculations is also provided. As a case study, total risk values are calculated for conformity assessment of concentration of total suspended particulate matter (TSPM) in ambient air from three independent stone quarries in Israel. In this

study TSPM contributed by the  $i$ -th quarry,  $i = 1, 2, 3$ , is considered as the  $i$ -th pollutant. While particular risk values of false decisions on conformity of the  $i$ -th TSPM concentration, evaluated earlier (Kuselman et al., 2012a), were related to each  $i$ -th pollutant ( $i$ -th quarry) separately, the total risk values discussed below allow characterization of conformity of the TSPM concentration in the region of the quarries as a whole. That is important as for the Regulator (the Ministry of Environmental Protection, Online) protecting the inhabitants' quality of life in the area surrounding the quarries, as for the Manufacturers Association (Online) acting in the interests of the stone producers in the country.

## 2. Methods

### 2.1. Raw data

#### 2.1.1. Test method and likelihood functions

A measured TSPM concentration in ambient air  $c_{im}$ ,  $\text{mg m}^{-3}$ , is an averaged mass of particles with aerodynamic diameters of  $100 \mu\text{m}$  or less collected from the air drawn through a filter in a high-volume sampler over the sampling period of the test in proximity to the  $i$ -th stone quarry. The testing was organized at a distance of (1-3) km from each quarry during the quarry' work. Each test lasted 24 hours for collection of particles from about  $2000 \text{ m}^3$  of air (EPA IO-2.1, 1999). The distribution of the test/measurement results  $c_{im}$  at the actual concentration  $c_i$  was found to be normal with standard deviation equal to the standard measurement uncertainty  $u_i =$



0.07  $c_{im}$  and mean equal to  $c_i$  (Kuselman et al., 2012a). Corresponding likelihood functions are normal probability density functions (pdfs):

$$f(c_{im}|c_i) = \frac{1}{u_i\sqrt{2\pi}} \exp\left[-\frac{(c_{im} - c_i)^2}{2u_i^2}\right]. \quad (3)$$

### 2.1.2. Database and prior distributions of actual concentration values

The database of 496 test results obtained during a year and described in the work of Kuselman et al. (2012a) is considered again in the present paper. On the basis of the analysis of variances (ANOVA), it was shown that the wind from the desert did not influence the test results significantly, whereas anthropogenic contributions to TSPM concentration were dominant. No correlation among test results for different quarries was observed. The theoretical distributions of actual values of TSPM concentration  $c_i$ , fitting successfully the data collected close to quarry  $i$ , were lognormal distributions, used in the following as prior pdfs:

$$f(c_i) = \frac{1}{c_i\sigma_i\sqrt{2\pi}} \exp\left[-\frac{(\ln c_i - \mu_i)^2}{2\sigma_i^2}\right], \quad (4)$$

where standard deviations  $\sigma_i$  and means  $\mu_i$  are for the first quarry ( $i = 1$ ) 0.434 and -2.326, respectively, on the logarithmic scale; for the second quarry ( $i = 2$ ) they are 0.280 and -2.031, respectively; and for the third quarry  $\sigma_3 = 0.403$  and  $\mu_3 = -2.338$ .

## 2.2. Regulation and acceptance limits

There are national regulations of ambient air quality including upper regulation limits  $T_{Ui}$  for TSPM concentration depending on the period of sampling. In Israel,  $T_{Ui} = 0.200 \text{ mg m}^{-3}$  for 24 hours, i.e. the same limit value is valid for any location in the country, also close to the  $i$ -th quarry.

Besides the regulation limit, a lower/stricter acceptance limits  $A_i$  could be applied for the test results with the purpose of decreasing the underestimation (inhabitant's) risks due to measurement uncertainty  $u_i$ . In such a case, the decision rules (is the air conforming or not?) are based on comparing the test results with the relevant  $i$ -th acceptance limit (JCGM 106, 2012; Ellison and Williams, 2007). The acceptance limits in the present study are taken as coincidental with the regulation limits.

### 2.3. Particular risks of under- and overestimation

#### 2.3.1. Particular specific risks

The particular specific risks of the pollutant concentration under- and overestimation are respectively

$$R_{ci(u)}^* = \int_{T_{Ui}}^{\infty} f(c_i|c_{im}) dc_i, \text{ for } c_{im} \leq T_{Ui}, \text{ and} \quad (5a)$$

$$R_{ci(o)}^* = \int_0^{T_{Ui}} f(c_i|c_{im}) dc_i, \text{ for } c_{im} > T_{Ui}, \quad (5b)$$

where  $f(c_i|c_{im})$  is the posterior pdf for the actual value of the TSPM concentration  $c_i$  contributed by the  $i$ -th quarry, given the measurement result near the quarry  $c_{im}$ . From Bayes Law the posterior pdf is

$$f(c_i|c_{im}) = f(c_{im}|c_i)f(c_i) / \int_{-\infty}^{\infty} f(c_{im}|c_i)f(c_i) dc_i, \quad (5c)$$

where  $f(c_{im}|c_i)$  is the likelihood function by eqn (3) and  $f(c_i)$  is the prior pdf by eqn (4).

### 2.3.2. Particular global risks

The global risks of  $c_i$  under- and overestimation related to the TSPM regulation limit  $T_{Ui}$ , are respectively

$$R_{ci(u)} = \int_{T_{Ui}}^{\infty} \int_0^{T_{Ui}} f(c_{im}|c_i)f(c_i) dc_{im}dc_i, \quad (6a)$$

$$R_{ci(o)} = \int_0^{T_{Ui}} \int_{T_{Ui}}^{\infty} f(c_{im}|c_i)f(c_i) dc_{im}dc_i. \quad (6b)$$

### 2.3.3. Probabilities of an acceptable test result and a conforming actual concentration value

Probability  $P(C_i)$  of a conforming test/measurement result for the  $i$ -th pollutant ( $c_{im} \leq A_i = T_{Ui}$ ) is calculated by marginalization of the joint pdf of the measurement results and the actual values of TSPM concentration:

$$P(C_i) = \int_0^\infty \int_0^{T_{Ui}} f(c_{im}|c_i) f(c_i) dc_{im} dc_i . \quad (7a)$$

181

182 Probability  $P(\bar{B}_i)$  that the actual concentration value for the  $i$ -th pollutant is conforming  
183 ( $c_i \leq T_{Ui}$ ) is calculated as:

184

$$P(\bar{B}_i) = \int_0^{T_{Ui}} f(c_i) dc_i . \quad (7b)$$

186

187 Note that the probability  $P(\bar{B}_i)$  of a conforming actual (true) value  $c_i$  in eqn (7b) does not  
188 depend on the measurement result  $c_{im}$  by definition. However, the vice versa holds: probability  
189  $P(C_i)$  of a conforming measurement result  $c_{im}$  by eqn (7a) does depend on the relevant actual  
190 value  $c_i$ .

191

### 192 3. Modeling and calculation

193

#### 194 3.1. Total risks of overestimation

195

##### 196 3.1.1. Events

197

198 Define the following events possible during testing concentrations of two or more pollutants  
199 in an environmental compartment:

- 200 ■  $\bar{B}_i$ : the actual concentration  $c_i$  of pollutant  $i$  does not exceed its regulation limit  $T_{Ui}$ ;  
201 probability of this event  $P(\bar{B}_i)$  is defined by formula (7b).

- 202     ▪  $\bar{B}$ : the actual concentration values  $c_i$  for any  $i$  do not exceed their own regulation limits
- 203      $T_{Ui}$ ,  $\bar{B} = \bar{B}_1 \cap \bar{B}_2 \cap \dots \cap \bar{B}_n$ ; probability of this event is  $P(\bar{B}) = \prod_{i=1}^n P(\bar{B}_i)$ , if  $\bar{B}_i$  are
- 204     mutually independent.
- 205     ▪  $B_i$ : the actual concentration  $c_i$  of pollutant  $i$  exceeds  $T_{Ui}$ , i.e. violates it; probability of this
- 206     event is  $P(B_i) = 1 - P(\bar{B}_i)$ .
- 207     ▪  $B$ : the actual concentration values  $c_i$  of one or more pollutants exceed their regulation
- 208     limits  $T_{Ui}$ ,  $B = B_1 \cup B_2 \cup \dots \cup B_n$ ; probability of this event is  $P(B) = 1 - P(\bar{B}) = 1 -$
- 209      $\prod_{i=1}^n P(\bar{B}_i)$ .
- 210     ▪  $C_i$ : the test result  $c_{im}$  for  $i$ -th pollutant does not exceed its acceptance limit  $A_i$ ; probability
- 211     of this event  $P(C_i)$  is defined by formula (7a).
- 212     ▪  $C$ : the test results  $c_{im}$  for any  $i$  do not exceed their own acceptance limits  $A_i$ ,  $C = C_1 \cap$
- 213      $C_2 \cap \dots \cap C_n$ ; probability of this event is  $P(C) = \prod_{i=1}^n P(C_i)$ , if  $C_i$  are mutually
- 214     independent.
- 215     ▪  $\bar{C}_i$ : the test result  $c_{im}$  for  $i$ -th pollutant exceeds its acceptance limit  $A_i$ , i.e. such  $c_{im}$  is an
- 216     out-of-specification test result (Kuselman et al., 2012b) as  $A_i = T_{Ui}$  in the present study;
- 217     probability of this event is  $P(\bar{C}_i) = 1 - P(C_i)$ .
- 218     ▪  $\bar{C}$ : one or more test results  $c_{im}$  exceed their own  $A_i$ ,  $\bar{C} = \bar{C}_1 \cup \bar{C}_2 \cup \dots \cup \bar{C}_n$ ; probability of
- 219     this event is  $P(\bar{C}) = 1 - P(C) = 1 - \prod_{i=1}^n P(C_i)$ .

### 221 3.1.2. Total specific risk

222

223     When a specified environmental compartment is tested concerning concentrations of three

224     pollutants, the total specific risk of overestimation  $R_{\text{total(o)}}^*$  is the probability that the actual

concentrations of all pollutants in this compartment conform to their regulation limits ( $\bar{B} = \bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3$ ), whereas one or more test/measurement results  $c_{1m}$ ,  $c_{2m}$  and  $c_{3m}$  exceed their acceptance limits. This event can occur when:

a) Just one measurement result out of the three, for example  $c_{1m}$  without losing generality, exceeds its acceptance limit, while the actual concentration  $c_1$  does not exceed the regulation limit. In this case, the actual concentration  $c_1$  will be overestimated. Hence, the total risk that the compartment is falsely considered as not conforming is equal to the particular specific risk concerning the first pollutant:  $R_{\text{total(o)}}^* = P(\bar{B}_1 | c_{1m})$ .

b) Two measurement results, e.g.  $c_{1m}$  and  $c_{2m}$ , exceed their acceptance limits. The total risk is  $R_{\text{total(o)}}^* = P(\bar{B}_1 \cap \bar{B}_2 | c_{1m}, c_{2m})$ .

c) All the three measurement results exceed their acceptance limits. The total risk is  $R_{\text{total(o)}}^* = P(\bar{B} | c_{1m}, c_{2m}, c_{3m}) = P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 | c_{1m}, c_{2m}, c_{3m})$ .

If the events  $\bar{B}_i$  are conditionally independent, i.e. independent of the measurement results  $c_{im}$ , the total specific risk in each of the three considered situations is, respectively:

$$\text{a) } R_{\text{total(o)}}^* = P(\bar{B}_1 | c_{1m}), \quad (8a)$$

$$\text{b) } R_{\text{total(o)}}^* = \prod_{i=1}^2 P(\bar{B}_i | c_{im}), \quad (8b)$$

$$\text{c) } R_{\text{total(o)}}^* = \prod_{i=1}^3 P(\bar{B}_i | c_{im}), \quad (8c)$$

where  $P(\bar{B}_i | c_{im}) = R_{ci(o)}^*$  by formula (5b).

For any number  $n$  of pollutants,  $v \leq n$  of which are characterized by the measurement results exceeding their acceptance limits, the total specific risk of overestimation is

$$R_{\text{total(o)}}^* = \prod_{i=1}^v R_{ci(o)}^* \quad (9)$$

249

250 Note again that  $R_{ci(o)}^*$  in eqn (9) are related to the out-of-specification measurement results of  
 251 concentrations of the pollutants, sorted as the first  $v$  from all  $n$  pollutants under control.

252 From eqn (9) it follows that any one of  $v$  particular specific risk of overestimation  $R_{ci(o)}^*$  equal  
 253 to zero will lead to  $R_{\text{total(o)}}^* = 0$ . That occurs when the actual concentration of the  $i$ -th pollutant  
 254  $c_i$  exceeds/violates the regulation limit unquestionably ( $c_i > T_{Ui}$ ) at a given measurement result  
 255  $c_{im} > T_{Ui}$  for this pollutant. In such a case, which does not depend on measurement results of  
 256 concentrations of the other pollutants, the compartment as a whole is certainly not conforming.  
 257 Therefore, the producer(s) should take action to reduce the  $i$ -th pollutant concentration and/or to  
 258 pay a fine.

259 In the opposite case of a particular specific risk value  $R_{ci(o)}^* = 1$ , although  $c_{im}$  exceeds its  
 260 acceptance limit, the actual concentration  $c_i$  certainly conforms. Such  $R_{ci(o)}^*$  would not influence  
 261 the total specific risk  $R_{\text{total(o)}}^*$  by eqn (9). In this case, the number  $n$  of pollutants is *de-facto*  
 262 decreased by one.

263 Another property of eqn (9) is reduction of  $R_{\text{total(o)}}^*$  with increasing number  $v$  of pollutants  
 264 for which the measurement results are out-of-specification. The logic is that the more such  
 265 measurement results, the smaller is the total probability of the overestimation. Thus, the greater  
 266 is the probability that the compartment as a whole does not conform.

267 Note also that the model used in the work of Subaric-Leitis (2010) and adopted later in the  
 268 EURAMET guide (Pendril et al., 2015) leads to an expression equivalent to eqn (9) when the  
 269 variables (concentrations of the pollutants in our task) are independent, hence validating the  
 270 model proposed in the present work.

### 3.1.3. Total global risk

Particular global risk  $R_{ci(o)}$  of overestimation for the  $i$ -th pollutant ( $i = 1, 2, 3$ ) is the probability of false nonconformance when the corresponding test result exceeds its acceptance limit  $A_i$ , while the actual value does not exceed the regulation limit  $T_{Ui}$ :

$$R_{ci(o)} = P(\bar{B}_i \cap \bar{C}_i). \quad (10)$$

The total global risk  $R_{total(o)}$  of overestimation is the risk of having the actual concentrations of the three pollutants within their regulation limits  $T_{Ui}$ , when at least one of test results are outside its acceptance limits (that is outside the three-dimensional domain  $A_1 \times A_2 \times A_3$ ), i.e.

$$R_{total(o)} = P(\bar{B} \cap \bar{C}), \text{ where}$$

$$\bar{B} \cap \bar{C} = \bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap (\bar{C}_1 \cup \bar{C}_2 \cup \bar{C}_3) = (\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1) \cup (\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_2) \cup (\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_3). \quad (11)$$

The total global risk of overestimation is thus:

$$R_{total(o)} = P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1) + P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_2) + P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_3) - P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1 \cap \bar{C}_2) - P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1 \cap \bar{C}_3) - P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_2 \cap \bar{C}_3) + P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1 \cap \bar{C}_2 \cap \bar{C}_3). \quad (12)$$



Whenever  $\bar{B}_1$ ,  $\bar{B}_2$  and  $\bar{B}_3$ , as well as  $\bar{C}_1$ ,  $\bar{C}_2$ , and  $\bar{C}_3$ , are mutually independent, events  $\bar{B}_1 \cap \bar{C}_1$ ,  $\bar{B}_2 \cap \bar{C}_2$  and  $\bar{B}_3 \cap \bar{C}_3$  are also independent and equation (12) can be rewritten using notation (10) in the following way:

$$R_{\text{total(o)}} = P(\bar{B}_2)P(\bar{B}_3)R_{c1(o)} + P(\bar{B}_1)P(\bar{B}_3)R_{c2(o)} + P(\bar{B}_1)P(\bar{B}_2)R_{c3(o)} - P(\bar{B}_3)R_{c1(o)}R_{c2(o)} - P(\bar{B}_2)R_{c1(o)}R_{c3(o)} - P(\bar{B}_1)R_{c2(o)}R_{c3(o)} + R_{c1(o)}R_{c2(o)}R_{c3(o)}. \quad (13)$$

Note that eqn (13) is similar to eqn (2) for the total global risk of underestimation. However, it involves probabilities of different events and different particular risks.

In general, for any number  $n$  of pollutants

$$R_{\text{total(o)}} = \sum_{i=1}^n (\prod_{l \neq i} P(\bar{B}_l)) R_{ci(o)} - \sum_{i=1}^n \sum_{j>i} (\prod_{l \neq i,j} P(\bar{B}_l)) (\prod_{q=i,j} R_{cq(o)}) + \sum_{i=1}^n \sum_{j>i} \sum_{k>j} (\prod_{l \neq i,j,k} P(\bar{B}_l)) (\prod_{q=i,j,k} R_{cq(o)}) + \dots + (-1)^{n-2} \sum_{i=1}^n P(\bar{B}_i) (\prod_{q \neq i} R_{cq(o)}) + (-1)^{n-1} \prod_{q=1}^n R_{cq(o)}, \quad (14)$$

where  $i, j, k, l$  and  $q$  are subscripts of the pollutant in the range  $(1, \dots, n)$ .

### 3.2. Calculation

When the likelihood function is a normal distribution and the prior pdf is lognormal, the posterior pdf cannot be easily described by an analytical closed form. Therefore, the posterior pdf was obtained by numerical integration (and subsequent normalization) of the product of the prior and the likelihood. The under- and overestimation particular risks were calculated as the fraction of the (approximated) posterior pdf lying outside/inside the tolerance limit, respectively.

Core code developed in R programming environment for calculation of the risks is reported in Annex A. Calculation of total specific risks of under- and overestimation by eqns (1) and (8), respectively, using corresponding particular specific risk values by eqns (5), is shown in Section A-1. Time spent for calculation of the total specific risks with a regular PC (Intel® Core™ i5-3470 Processor, CPU @ 3.20 GHz, Windows 7 Professional 64 bit) is about one second. While increasing (doubling, for example) the number of the involved components does not affect the calculation time, decreasing the numerical integration parameter (stepsize) from 0.001 to 0.0001, increases the execution time up to 6 seconds.

Calculation of total global risks of under- and overestimation by eqns (2) and (13), respectively, using particular global risk values by eqns (6), probabilities of conforming measurement results by eqn (7a) and probabilities of conforming actual concentration values by eqn (7b), is detailed in Section A-2. Time spent for calculation of the total global risks with the same PC is about 5 seconds. In this case, doubling the number of components doubles the required time, whereas decreasing the integration parameter (step) from 0.00001 to 0.000001 increases the computational time up to about 37 seconds.

#### 4. Results and discussion

#### 4.1. Total specific risks of under- and overestimation

Dependence of the total specific risks of underestimation of TSPM concentration in air on the measurement results  $c_{im}$  is demonstrated in Fig. 2. A case when only the first quarry is active and the total risk  $R_{total(u)}^*$  equals to the particular risk  $R_{c1(u)}^*$ , is shown in Fig. 2a by solid line 1.

Dotted lines 3 and 2 point a measured TSPM concentration  $c_{1m} = 0.194 \text{ mg m}^{-3}$  and corresponding risk value  $R_{c1(u)}^* = 0.211$ , as an instance. One can see in Fig. 2a that  $R_{c1(u)}^*$  is close to zero (negligible) at  $c_{1m} < 0.170 \text{ mg m}^{-3}$ , however significantly increasing with  $c_{1m}$  approaching the tolerance limit  $T_{U1} = 0.200 \text{ mg m}^{-3}$ .

A case when only the second and the third quarries are active, is represented in Fig. 2b, where the total risk,  $R_{total(u)}^*$ , shown as a surface, depends on both  $c_{2m}$  and  $c_{3m}$  in the range  $[0.010, 0.200] \text{ mg m}^{-3}$ . The surface lies mostly on the bottom of the three-dimensional region where  $R_{total(u)}^*$  is close to zero, as in Fig. 2a, increasing with  $c_{2m}$  and  $c_{3m}$  approaching their tolerance limits  $T_{U1} = T_{U2} = 0.200 \text{ mg m}^{-3}$ . When both  $c_{2m}$  and  $c_{3m}$  simultaneously approach  $0.200 \text{ mg m}^{-3}$ , this leads to a ‘protuberance’ in the total risk surface.

The same dependence of  $R_{total(u)}^*$  on  $c_{2m}$  and  $c_{3m}$  is observed when all the three quarries are active simultaneously, but  $c_{1m} < 0.170 \text{ mg m}^{-3}$ : the contribution of the particular risk  $R_{c1(u)}^*$  to the total one in such a case is negligible as shown in Fig. 2a. For comparison, Fig. 2c illustrates a scenario when all the three quarries are active and  $R_{total(u)}^*$  - the surface - is depending on  $c_{2m}$  and  $c_{3m}$  in the range  $[0.010, 0.200] \text{ mg m}^{-3}$  as in Fig. 2b, whereas  $c_{1m} = 0.194 \text{ mg m}^{-3}$ . Fig. 2c seems very similar to Fig. 2b. However, the color scales of the  $R_{total(u)}^*$  surfaces are different, since the scale in Fig. 2c is greater because of the significant contribution of  $R_{c1(u)}^* = 0.211$  at  $c_{1m} = 0.194 \text{ mg m}^{-3}$  (indicated in Fig 2a by dotted lines).

Fig. 3 Dependence of the total specific risks of overestimation of the actual TSPM concentration in air on measurement results, when they are out-of-specification ( $c_{im} > T_{Ui}$ ), is detailed in Fig. 3.

A case when only the first quarry is active, and the total risk  $R_{total(o)}^*$  is equal to the particular risk  $R_{c1(o)}^*$ , is shown in Fig. 3a by solid line 1. Dotted lines 3 and 2 point a measured TSPM concentration  $c_{1m} = 0.250 \text{ mg m}^{-3}$  and corresponding risk value  $R_{c1(o)}^* = 0.008$ , as an example. Naturally, the risk of overestimation increases as  $c_{1m}$  approaches  $0.200 \text{ mg m}^{-3}$  (the tolerance limit), and is close to zero for  $c_{1m} > 0.260 \text{ mg m}^{-3}$ .

The case when only the second and the third quarries are active, as in Fig 2b, and  $R_{total(o)}^*$  value depending on both  $c_{2m}$  and  $c_{3m}$  in the range  $[0.210, 0.300] \text{ mg m}^{-3}$ , is shown in Fig. 3b. The maximum  $R_{total(o)}^*$  value is observed as  $c_{2m}$  and  $c_{3m}$  near the tolerance limit simultaneously.

Fig. 3c illustrates a case when all the three quarries are active, as in Fig. 2c, but  $c_{1m} = 0.250 \text{ mg m}^{-3}$ . The scale of the  $R_{total(u)}^*$  surface, shown by the color bar, is two orders less than in Fig. 3b. The reason is that the total risk of overestimation, defined as a product of the three particular risks, is influenced by the contribution of  $R_{c1(o)}^* = 0.008$  at  $c_{1m} = 0.250 \text{ mg m}^{-3}$  (indicated in Fig 3a by dotted lines). In other words, if an out-of-specification measurement result is significantly greater than the tolerance limit, the probability of violation of the regulation is high and the particular risk of overestimation is low. Therefore the total specific risk of overestimation is low also.

#### 4.2. Total global risks of under- and overestimation

The particular global risks of underestimation  $R_{c1(u)} = 0.006$ ,  $R_{c2(u)} = 0.010$  and  $R_{c3(u)} = 0.005$  obtained here are equal to the values published earlier (Kuselman et al., 2012a). They are

used as a part of the validation process of the current calculations. The probabilities of conforming measurement results are  $P(C_1) = 0.949$ ,  $P(C_2) = 0.929$  and  $P(C_3) = 0.963$ . The total risk of underestimation, evaluated in the present work for the first time, is  $R_{\text{total}(u)} = 0.019$ , hence greater than the particular risk contributed by each quarry.

The particular global risks of overestimation are  $R_{c1(o)} = 0.007$ ,  $R_{c2(o)} = 0.015$  and  $R_{c3(o)} = 0.006$ . They are also equal to those published by Kuselman et al. (2012a). The probabilities of conforming actual concentration values calculated are  $P(\bar{B}_1) = 0.951$ ,  $P(\bar{B}_2) = 0.934$  and  $P(\bar{B}_3) = 0.965$ . The total risk of overestimation, evaluated in the present work for the first time as well, is  $R_{\text{total}(o)} = 0.026$ , again greater than each  $R_{ci(o)}$ .

The total risk of overestimation  $R_{\text{total}(o)}$  exceeds the total risk of underestimation  $R_{\text{total}(u)}$ , which implies that there is a reasonable balance between the requirements of an inhabitant's quality of life and the producer's expenditure on environmental protection.

## 5. Conclusions

Quantification of risks of false decisions in conformity assessment of an environmental compartment due to measurement uncertainty of concentrations of two or more pollutants, is developed. Even if the assessment of conformity for each pollutant in the compartment is successful, the total probability of a false decision concerning the compartment as a whole might still be significant.

A model of the total probability of a false decision, formulated on the basis of the law of total probability, is used for a study of test results of total suspended particulate matter concentration in ambient air from three independent stone quarries in Israel. Total probabilities of

underestimation of the particulate matter concentration (total risk of the inhabitants) and overestimation (total risk of the stone producers) are evaluated as a combination of the particular risks of air conformity assessment near to each quarry.

It is shown that the total global risk of underestimation of the particulate matter concentration is smaller than the total risk of its overestimation. That is a reasonable balance between the requirements of an inhabitant's quality of life and the producer's expenditure on environmental protection.

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## Appendix A. Core of the R code

### A-1. Calculation of the total specific risks

```
#####  
# Specific risks #  
#####  
  
# Input data for the quarries  
mu1 = -2.326      # Prior location parameter for Q1  
mu2 = -2.031      # Prior location parameter for Q2  
mu3 = -2.338      # Prior location parameter for Q3  
sigma1 = 0.434     # Prior scale parameter for Q1  
sigma2 = 0.280     # Prior scale parameter for Q2  
sigma3 = 0.403     # Prior scale parameter for Q3
```

```

436 Rsigmam = 0.07      # Relative measurement uncertainty
437 TU = 0.2           # Tolerance limit
438
439 # Settings for numerical integrations
440 stepsize <- 0.001
441 obsvalues = seq(0.01,TU,stepsize)
442 postmean = rep(0,length(obsvalues))
443 poststd = rep(0,length(obsvalues))
444 Rspec1 = rep(0,length(obsvalues))
445 Rspec2 = rep(0,length(obsvalues))
446 Rspec3 = rep(0,length(obsvalues))
447 c = seq(0,0.5,stepsize)
448
449 #####
450 # Consumer specific risk for each observed value in [0.01, TU]
451 # Normal Likelihood and Lognormal prior
452
453 # Q1
454 i = 1
455 prior <- dlnorm(c, meanlog = mu1, sdlog = sigma1)
456 logprior <- log(prior)
457 for(obs in obsvalues)
458 {
459   loglik <- dnorm(obs, mean = c, sd = Rsigmam*obs, log = T)
460   logpos <- logprior + loglik
461   posterior <- exp(logpos)
462   posterior <- posterior/(sum(posterior)*stepsize)
463   postmean[i] <- sum(posterior*c)*stepsize
464   postvar <- sum(posterior*(c^2))*stepsize-postmean[i]^2
465   poststd[i] = sqrt(postvar)
466   Rspec1[i] = stepsize*sum(posterior[c>TU])
467   i = i+1
468 }
469
470 # Q2
471 i = 1
472 prior <- dlnorm(c, meanlog = mu2, sdlog = sigma2)
473 logprior <- log(prior)
474 for(obs in obsvalues)
475 {
476   loglik <- dnorm(obs, mean = c, sd = Rsigmam*obs, log = T)
477   logpos <- logprior + loglik
478   posterior <- exp(logpos)
479   posterior <- posterior/(sum(posterior)*stepsize)
480   postmean[i] <- sum(posterior*c)*stepsize
481   postvar <- sum(posterior*(c^2))*stepsize-postmean[i]^2

```

```

482   poststd[i] = sqrt(postvar)
483   Rspec2[i] = stepsize*sum(posterior[c>TU])
484   i = i+1
485   }
486
487   # Q3
488   i = 1
489   prior <- dlnorm(c, meanlog = mu3, sdlog = sigma3)
490   logprior <- log(prior)
491   for(obs in obsvalues)
492   {
493     loglik <- dnorm(obs, mean = c, sd = Rsigmam*obs, log = T)
494     logpos <- logprior + loglik
495     posterior <- exp(logpos)
496     posterior <- posterior/(sum(posterior)*stepsize)
497     postmean[i] <- sum(posterior*c)*stepsize
498     postvar <- sum(posterior*(c^2))*stepsize-postmean[i]^2
499     poststd[i] = sqrt(postvar)
500     Rspec3[i] = stepsize*sum(posterior[c>TU])
501     i = i+1
502   }
503
504   # Total specific consumer risk for the particular case obs1=obs2=obs3
505   Rtotu = Rspec1 + Rspec2 + Rspec3 - Rspec1*Rspec2 - Rspec1*Rspec3 - Rspec2*Rspec3 +
506   Rspec1*Rspec2*Rspec3
507
508   #####
509   # Producer specific risk for each observed value in [0.21, 0.3]
510
511   # Settings for numerical integrations
512   obsvalues = seq(0.21,0.3,stepsize)
513   postmean = rep(0,length(obsvalues))
514   poststd = rep(0,length(obsvalues))
515   Rspec1 = rep(0,length(obsvalues))
516   Rspec2 = rep(0,length(obsvalues))
517   Rspec3 = rep(0,length(obsvalues))
518
519   # Q1
520   i = 1
521   prior <- dlnorm(c, meanlog = mu1, sdlog = sigma1)
522   logprior <- log(prior)
523   for(obs in obsvalues)
524   {
525     loglik <- dnorm(obs, mean = c, sd = Rsigmam*obs, log = T)
526     logpos <- logprior + loglik
527     posterior <- exp(logpos)

```



```

528 posterior <- posterior/(sum(posterior)*stepsize)
529 postmean[i] <- sum(posterior*c)*stepsize
530 postvar <- sum(posterior*(c^2))*stepsize-postmean[i]^2
531 poststd[i] = sqrt(postvar)
532 Rspec1[i] = stepsize*sum(posterior[c<=TU])
533 i = i+1
534 }
535
536 # Q2
537 i = 1
538 prior <- dlnorm(c, meanlog = mu2, sdlog = sigma2)
539 logprior <- log(prior)
540 for(obs in obsvalues)
541 {
542   loglik <- dnorm(obs, mean = c, sd = Rsigmam*obs, log = T)
543   logpos <- logprior + loglik
544   posterior <- exp(logpos)
545   posterior <- posterior/(sum(posterior)*stepsize)
546   postmean[i] <- sum(posterior*c)*stepsize
547   postvar <- sum(posterior*(c^2))*stepsize-postmean[i]^2
548   poststd[i] = sqrt(postvar)
549   Rspec2[i] = stepsize*sum(posterior[c<=TU])
550   i = i+1
551 }
552
553 # Q3
554 i = 1
555 prior <- dlnorm(c, meanlog = mu3, sdlog = sigma3)
556 logprior <- log(prior)
557 for(obs in obsvalues)
558 {
559   loglik <- dnorm(obs, mean = c, sd = Rsigmam*obs, log = T)
560   logpos <- logprior + loglik
561   posterior <- exp(logpos)
562   posterior <- posterior/(sum(posterior)*stepsize)
563   postmean[i] <- sum(posterior*c)*stepsize
564   postvar <- sum(posterior*(c^2))*stepsize-postmean[i]^2
565   poststd[i] = sqrt(postvar)
566   Rspec3[i] = stepsize*sum(posterior[c<=TU])
567   i = i+1
568 }
569
570 # Total specific producer risk for the particular case obs1=obs2=obs3
571 Rtoto = Rspec1*Rspec2*Rspec3
572

```

573 **A-2. Calculation of the total global risks**

574

```

575 #####
576 # Global risks #
577 #####
578
579 # Input data for the quarries
580 mu1 = -2.326      # Prior location parameter for Q1
581 mu2 = -2.031      # Prior location parameter for Q2
582 mu3 = -2.338      # Prior location parameter for Q3
583 sigma1 = 0.434    # Prior scale parameter for Q1
584 sigma2 = 0.280    # Prior scale parameter for Q2
585 sigma3 = 0.403    # Prior scale parameter for Q3
586 um = 0.07         # Relative measurement uncertainty
587 T = 0.2           # Tolerance limit
588 A = T             # Acceptance limit
589
590 # Consumer's risk Rc and the producer's risk Rp
591 # Normal Likelihood and Lognormal prior
592 # Initializations
593 step = 0.00001
594 etac = seq(T,10,step)      # Integral domain [T, infinity]
595 etap = seq(step,T,step)    # Integral domain [0, T]
596 etacinf = seq(step,10,step) # Integral domain [0, infinity]
597
598 # Q1
599 ymeanlogQ1 = mu1
600 ystdlogQ1 = sigma1
601 RcQ1 = sum( (pnorm((A-etac)/(um*etac)) - pnorm(-etac/(um*etac))) *
602 dlnorm(etac,ymeanlogQ1,ystdlogQ1) * step)
603 PC1 = sum( (pnorm((A-etacinf)/(um*etacinf)) - pnorm(-etacinf/(um*etacinf))) *
604 dlnorm(etacinf,ymeanlogQ1,ystdlogQ1) * step)
605 RpQ1 = sum( (1-pnorm((A-etap)/(um*etap))) * dlnorm(etap,ymeanlogQ1,ystdlogQ1) * step)
606 PBcompl1 = plnorm(T,ymeanlogQ1,ystdlogQ1)
607 c(RcQ1,RpQ1,PC1,PBcompl1)
608 # [1] 0.005769988 0.007368876 0.949038432 0.950637320
609
610 # Q2
611 ymeanlogQ2 = mu2
612 ystdlogQ2 = sigma2
613 RcQ2 = sum( (pnorm((A-etac)/(um*etac)) - pnorm(-etac/(um*etac))) *
614 dlnorm(etac,ymeanlogQ2,ystdlogQ2) * step)
615 PC2 = sum( (pnorm((A-etacinf)/(um*etacinf)) - pnorm(-etacinf/(um*etacinf))) *
616 dlnorm(etacinf,ymeanlogQ2,ystdlogQ2) * step)

```

```

617 RpQ2 = sum( (1- pnorm((A-etap)/(um*etap))) * dlnorm(etap,ymeanlogQ2,ystdlogQ2) * step)
618 PBcompl2 = plnorm(T,ymeanlogQ2,ystdlogQ2)
619 c(RcQ2,RpQ2,PC2,PBcompl2)
620 # [1] 0.01045913 0.01525355 0.92911792 0.93391234
621
622 # Q3
623 ymeanlogQ3 = mu3
624 ystdlogQ3 = sigma3
625 RcQ3 = sum( (pnorm((A-etac)/(um*etac)) - pnorm(-etac/(um*etac))) *
626 dlnorm(etac,ymeanlogQ3,ystdlogQ3) * step)
627 PC3 = sum( (pnorm((A-etacinf)/(um*etacinf)) - pnorm(-etacinf/(um*etacinf))) *
628 dlnorm(etacinf,ymeanlogQ3,ystdlogQ3) * step)
629 RpQ3 = sum( (1- pnorm((A-etap)/(um*etap))) * dlnorm(etap,ymeanlogQ3,ystdlogQ3) * step)
630 PBcompl3 = plnorm(T,ymeanlogQ3,ystdlogQ3)
631 c(RcQ3,RpQ3,PC3,PBcompl3)
632 # [1] 0.004602961 0.006233814 0.963053939 0.964684793
633
634 # TOTAL global consumer risk (underestimation risk)
635 c(PC1,PC2,PC3)
636 # [1] 0.9490384 0.9291179 0.9630539
637 c(RcQ1,RcQ2,RcQ3)
638 # [1] 0.005769988 0.010459133 0.004602961
639 Rtotu = PC2*PC3*RcQ1 + PC1*PC3*RcQ2 + PC1*PC2*RcQ3 - PC3*RcQ1*RcQ2 -
640 PC2*RcQ1*RcQ3 - PC1*RcQ2*RcQ3 + RcQ1*RcQ2*RcQ3
641 Rtotu # 0.01865286, for step = 0.00001
642
643 # TOTAL global producer risk (overestimation risk)
644 c(PBcompl1,PBcompl2,PBcompl3)
645 # [1] 0.9506373 0.9339123 0.9646848
646 c(RpQ1,RpQ2,RpQ3)
647 # [1] 0.007368876 0.015253553 0.006233814
648 Rtoto = PBcompl2*PBcompl3*RpQ1 + PBcompl1*PBcompl3*RpQ2 +
649 PBcompl1*PBcompl2*RpQ3 - PBcompl3*RpQ1*RpQ2 - PBcompl2*RpQ1*RpQ3 -
650 PBcompl1*RpQ2*RpQ3 + RpQ1*RpQ2*RcQ3
651 Rtoto # 0.0259206, for step = 0.00001
652

```

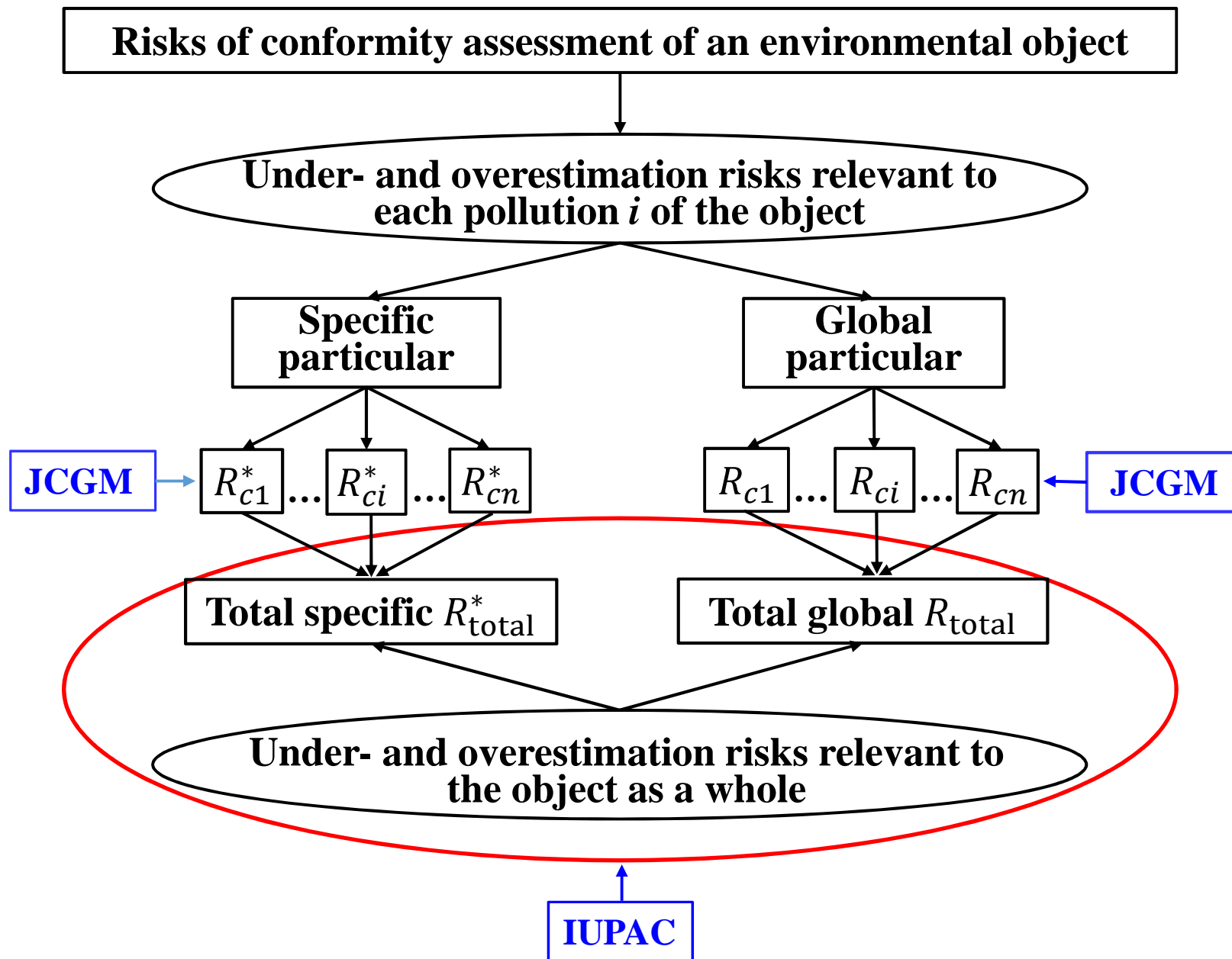
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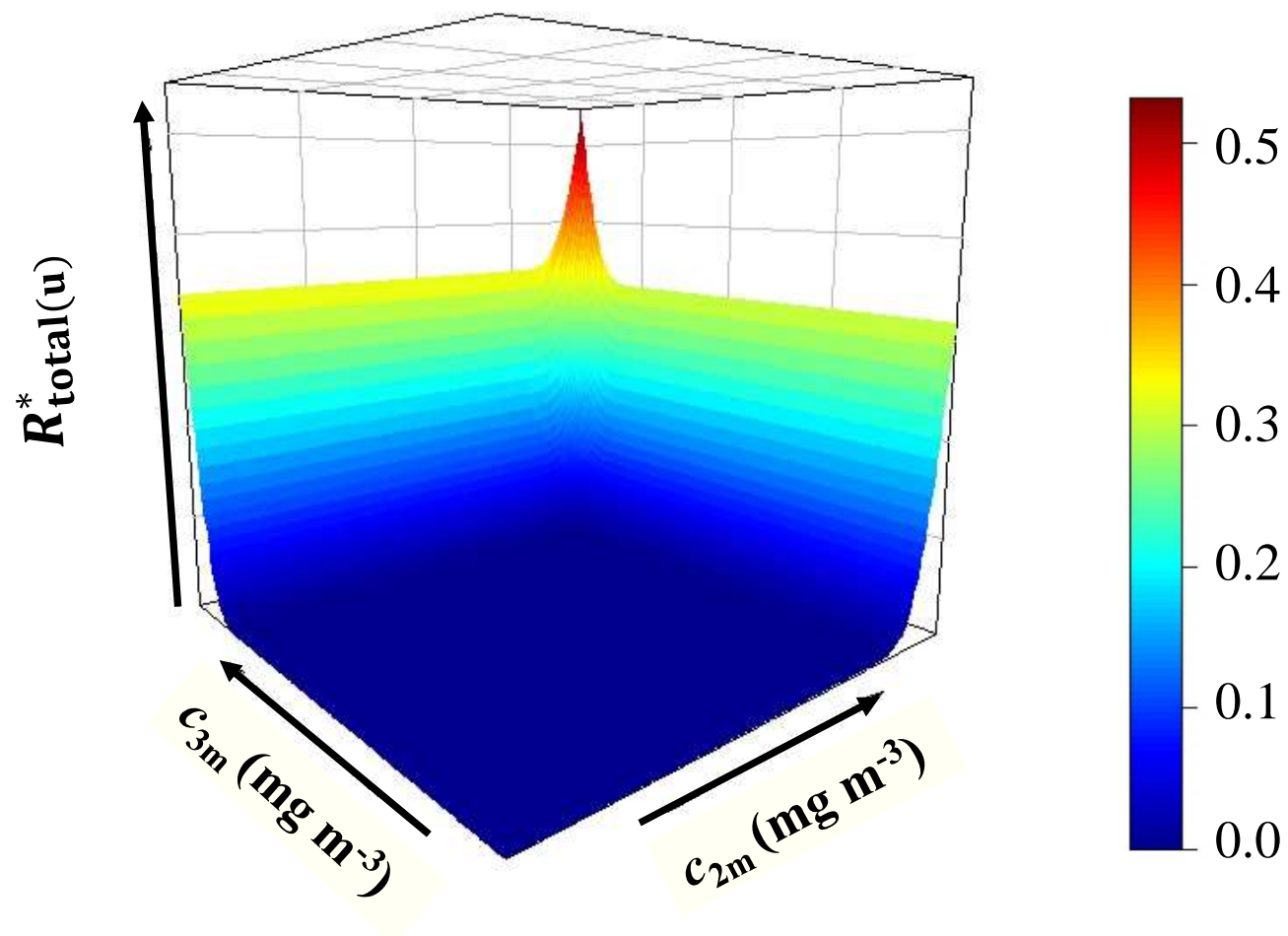
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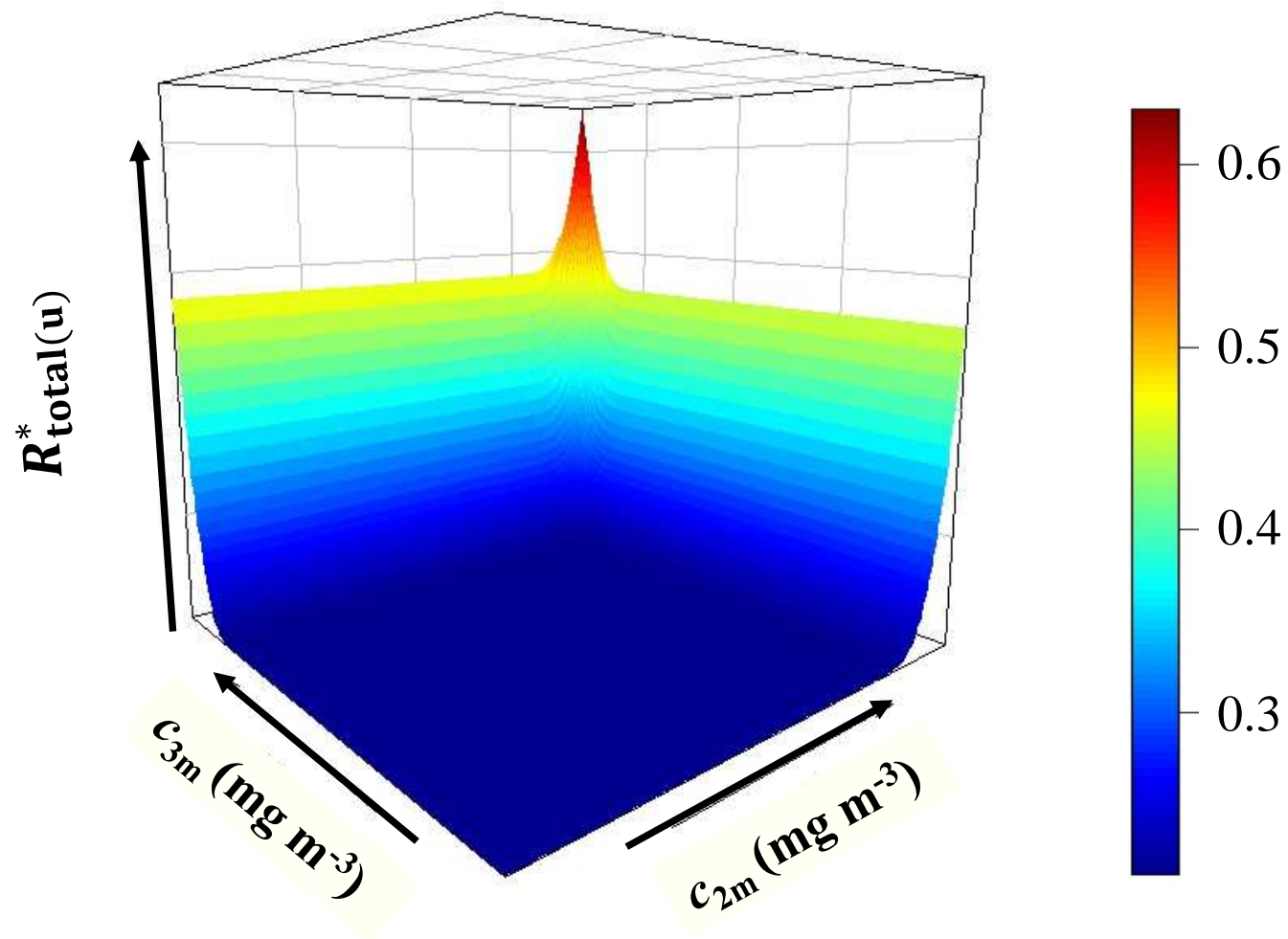


b)

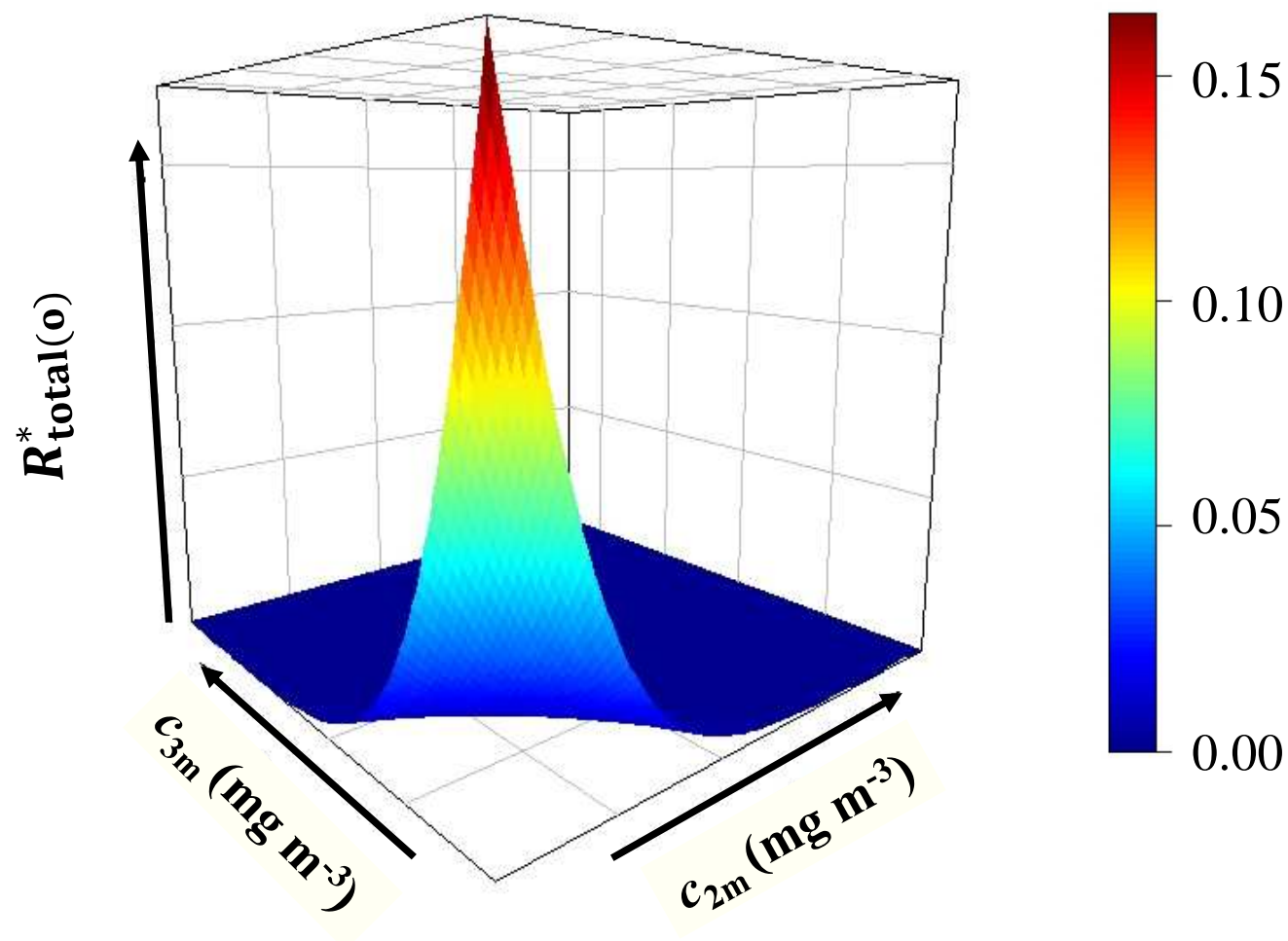




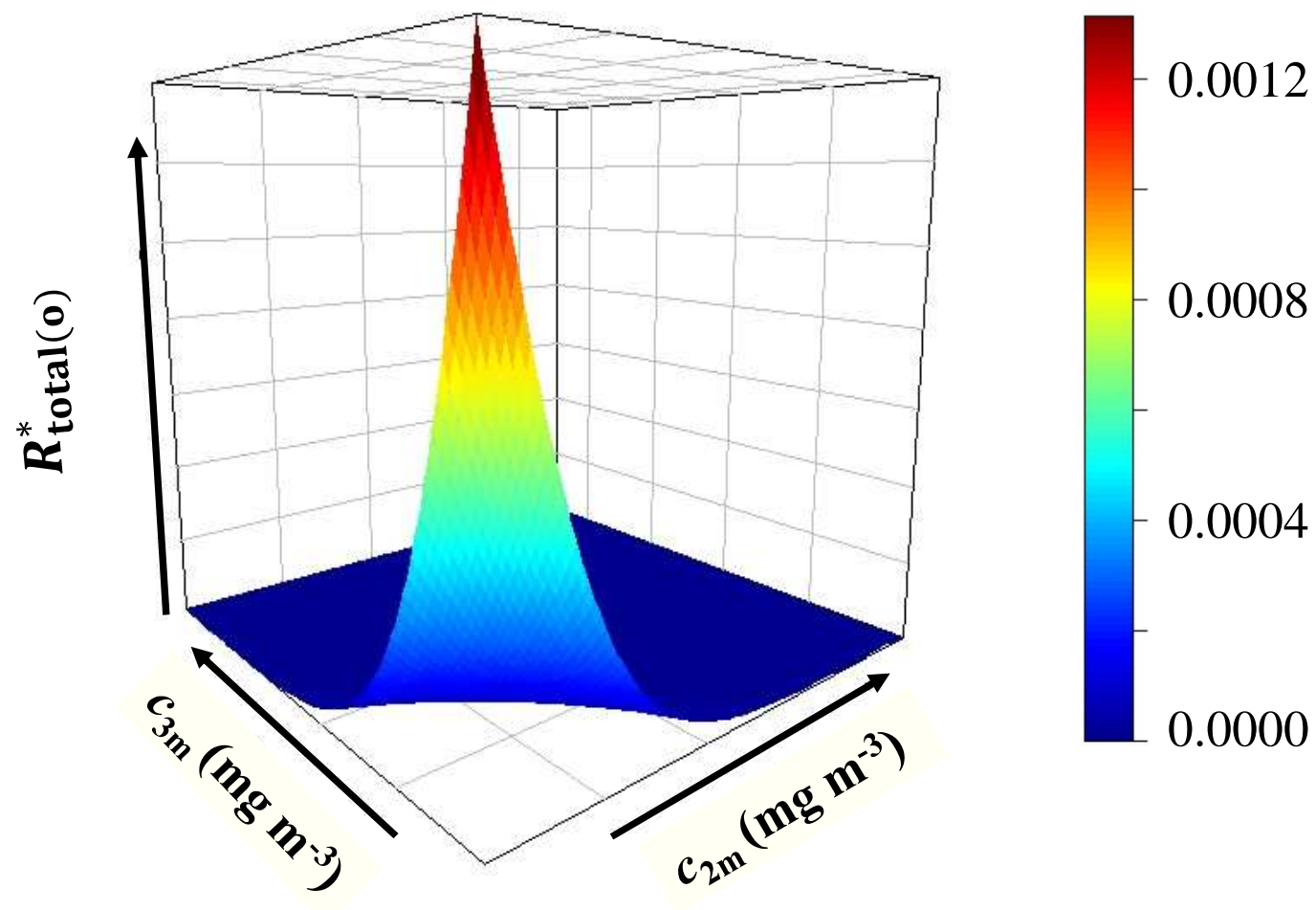
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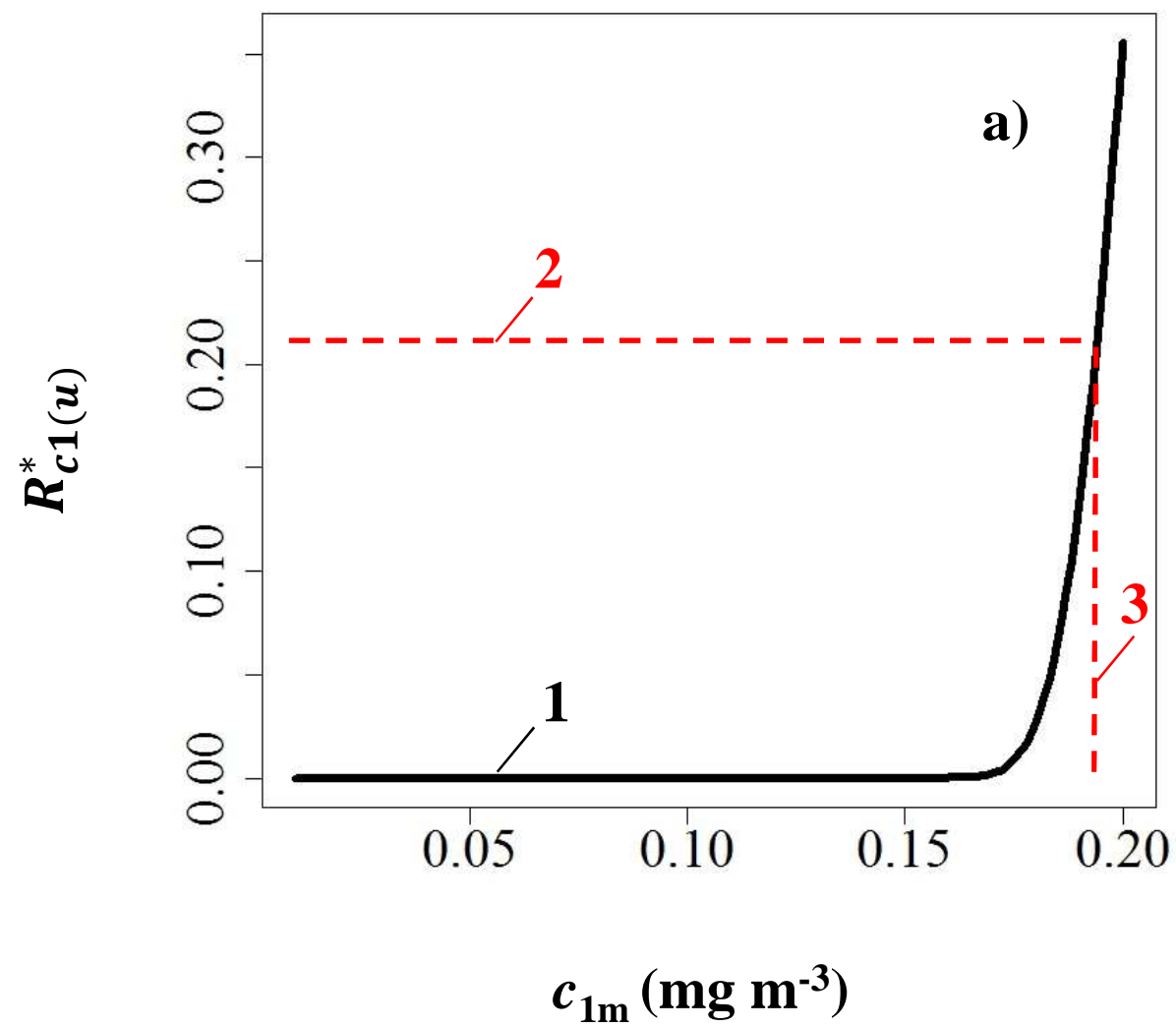


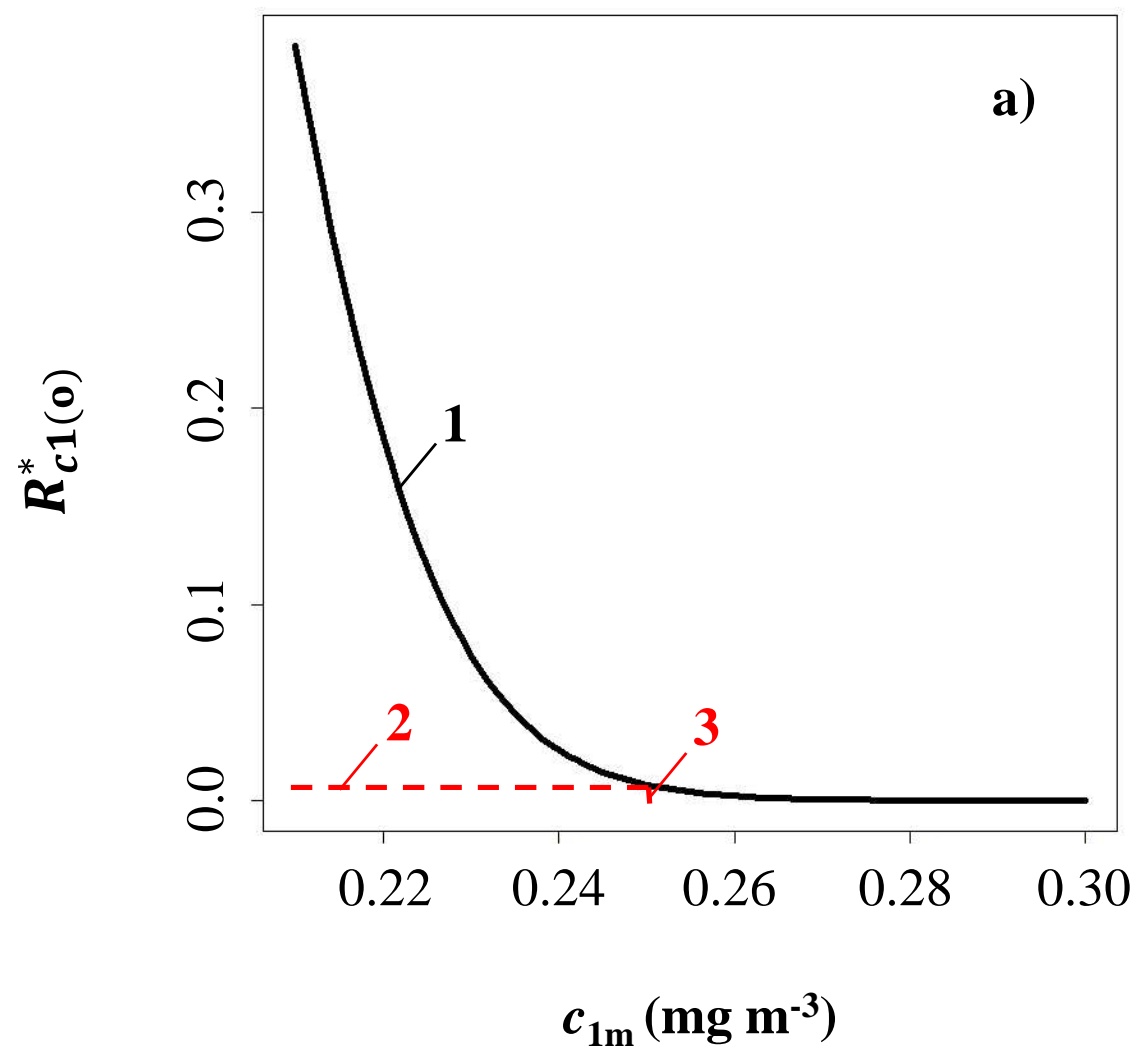
b)



c)







## Figure captions

**Fig. 1. Classification of the risks in conformity assessment of an environmental compartment due to measurement uncertainty.** Specific risk refers to a specified compartment in a certain location at a certain time, whereas global risk – to the population of such compartments. Particular risk (specific  $R_{ci}^*$  or global  $R_{ci}$ ) refers to  $i$ -th pollutant of the environmental compartment,  $i = 1, 2, \dots, n$ , according to the JCGM Guide 106 (2012); and total risk (specific  $R_{total}^*$  or global  $R_{total}$ ) – to the compartment as a whole. The total risk evaluation is the task of the IUPAC Project (2016), highlighted in the figure by an ellipse. These kinds of risks are relevant as for an underestimation of the pollutant concentration  $c_i$ , as for its overestimation, i.e. to the consumer' and producer's risks, respectively.

**Fig. 2. Dependence of the total specific risks of underestimation  $R_{total(u)}^*$  of TSPM concentration in air on the measurement results  $c_{im}$ .** Fig. 2a is for a case when only the first quarry is active and the total risk  $R_{total(u)}^*$  is equal to the particular risk  $R_{c1(u)}^*$ , shown by solid line 1. Dotted lines 3 and 2 point, as an example, a measured TSPM concentration  $c_{1m} = 0.194 \text{ mg m}^{-3}$  and corresponding risk value  $R_{c1(u)}^* = 0.211$ . Fig. 2b is for a case when only the second and the third quarries are active.  $R_{total(u)}^*$ , presented as a color surface, is depending on both  $c_{2m}$  and  $c_{3m}$  in the range  $[0.010, 0.200] \text{ mg m}^{-3}$ . The meaning of the color is the total risk value according to the color scale of the bar on the right side of the plot. Fig. 2c illustrates a case when all the three quarries are active and  $R_{total(u)}^*$  - the color surface - is depending on  $c_{2m}$  and  $c_{3m}$  in the range  $[0.010, 0.200] \text{ mg m}^{-3}$  as in Fig. 2b, but  $c_{1m} = 0.194 \text{ mg m}^{-3}$  (indicated in Fig 2a by dotted lines).

**Fig. 3. Dependence of the total specific risks of overestimation  $R_{\text{total(o)}}^*$  of the TSPM concentration in air on the measurement results  $c_{\text{im}}$ .** Fig. 3a is for a case when only the first quarry is active and the total risk  $R_{\text{total(o)}}^*$  is equal to the particular risk  $R_{c1(o)}^*$ , shown by solid line 1, while dotted lines 3 and 2 point, as an example, a measured TSPM concentration  $c_{1m} = 0.250 \text{ mg m}^{-3}$  and corresponding risk value  $R_{c1(o)}^* = 0.008$ . Fig. 3b is for a case when only the second and the third quarries are active, as in Fig 2b, and the total risk  $R_{\text{total(o)}}^*$  value is depending on both  $c_{2m}$  and  $c_{3m}$  in the range  $[0.210, 0.300] \text{ mg m}^{-3}$ . Fig. 3c illustrates a case when all the three quarries are active simultaneously as in Fig. 2c, but  $c_{1m} = 0.250 \text{ mg m}^{-3}$  (indicated in Fig 3a by dotted lines).

## HIGHLIGHTS

- Evaluation of total risks of false decisions on conformity of an environmental compartment is developed.
- The total risks due to measurement uncertainty of concentrations of two or more pollutants are considered.
- As a case study, the total risks are evaluated at control of total suspended particulate matter (TSPM) concentration in air.
- The study concerns three independent stone quarries as pollutant sources.
- The total probabilities of under- and overestimation of TSPM concentration in air are calculated.