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



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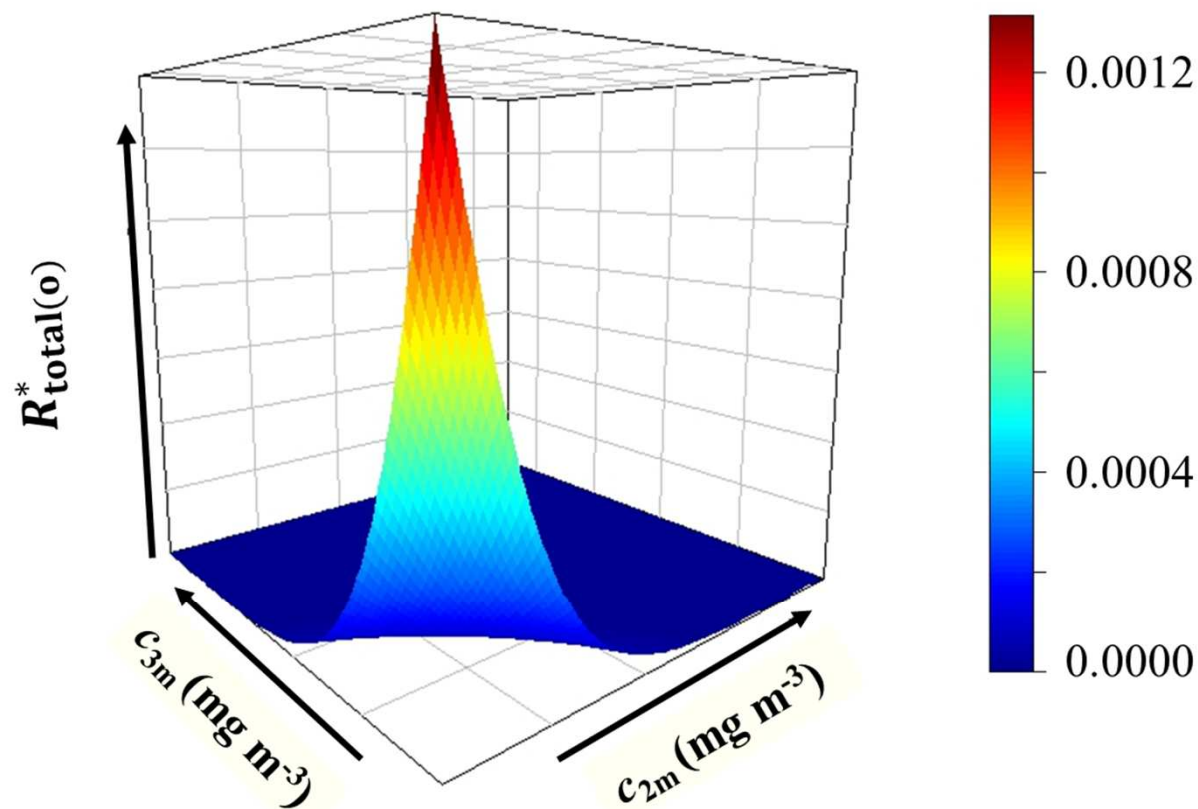
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Dependence of the total risk of overestimation $R_{total(o)}^*$ of suspended particulate matter concentration in ambient air on the measurement results c_{im} in proximity to the three quarries ($c_{1m} = 0.250$ mg m⁻³; c_{2m} and c_{3m} are varying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

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

4
5 **Francesca R. Pennechi ^a, Ilya Kuselman ^{b,*}, Ricardo J. N. B. da Silva ^c, D. Brynn Hibbert ^d**

6
7 ^a *Istituto Nazionale di Ricerca Metrologica (INRIM), Strada delle Cacce 91, 10135 Turin, Italy*

8 ^b *Independent Consultant on Metrology, 4/6 Yarehim St., 7176419 Modiin, Israel*

9 ^c *Centro de Química Estrutural, Faculdade de Ciências da Universidade de Lisboa, Edifício C8,*
10 *Campo Grande, 1749-016 Lisboa, Portugal*

11 ^d *School of Chemistry, UNSW Sydney, Sydney NSW 2052, Australia*

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14
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17 -----
18 * Corresponding author. Tel.: +972-50-6240466

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

20 4/6 Yarehim St., Modiin, 7176419 Israel

21

22

23 1. Introduction

24
25 Actual ('true') concentration c_i of the i -th pollutant, $i = 1, 2, \dots, n$, in an environmental
26 compartment, e.g. ambient air (Duursma and Carroll (1996); TIMBRE project, Online), should
27 not exceed a regulation or legal tolerance upper limit T_{Ui} . 'Concentration' is used here as a
28 generic term (Cvitaš, 1996; Tolhurst, 2005; Fuentes-Arderiu, 2013). Comparing a chemical
29 analytical test/measurement result c_{im} of the i -th pollutant concentration with the T_{Ui} value, one
30 should decide whether the compartment conforms to the regulation or not. Since any result c_{im}
31 has an associated measurement uncertainty (Ellison and Williams, 2012; Magnusson et al.,
32 2012), several kinds of risk of a false decision on conformity of the compartment may arise.

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

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

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

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

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

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

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

68

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

71

72 E.g., for all the particular specific risks $R_{ci(u)}^* = 0.05$, the total specific risk by formula (1) is

73 $R_{\text{total}}^* = 0.14$. Total global risk of underestimation for the three pollutants is:

74

$$75 \quad R_{\text{total}(u)} =$$

$$76 \quad P(C_2)P(C_3)R_{c1(u)} + P(C_1)P(C_3)R_{c2(u)} + P(C_1)P(C_2)R_{c3(u)} - P(C_3)R_{c1(u)}R_{c2(u)} -$$

$$77 \quad P(C_2)R_{c1(u)}R_{c3(u)} - P(C_1)R_{c2(u)}R_{c3(u)} + R_{c1(u)}R_{c2(u)}R_{c3(u)}, \tag{2}$$

78

79 where $P(C_i)$ is the probability that a measurement result c_{im} is acceptable, i.e. $c_{im} \leq T_{Ui}$. For

80 example, for the particular risks $R_{ci} = 0.05$ and probabilities $P(C_i) = 0.90$ for all i , formula (2)

81 gives $R_{\text{total}} = 0.12$.

82 General expressions for evaluating the total risk of underestimation for any number n of the

83 material components (or pollutants of an environmental compartment) are also provided in the

84 mentioned above reference. Treatment of correlated measurement results for total risk evaluation is

85 discussed in the paper by Kuselman et al. (2017b).

86 In the present paper, the total risk of overestimation (producer's risk) is formulated in the same

87 Bayesian framework for uncorrelated test results as it was applied in the previous work (Kuselman

88 et al., 2017a) for underestimation (consumer's risk). Core code developed in R programming

89 environment (the R project, Online) for corresponding calculations is also provided. As a case

90 study, total risk values are calculated for conformity assessment of concentration of total suspended

91 particulate matter (TSPM) in ambient air from three independent stone quarries in Israel. In this

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

100

101 **2. Methods**

102

103 **2.1. Raw data**

104

105 *2.1.1. Test method and likelihood functions*

106

107 A measured TSPM concentration in ambient air c_{im} , mg m^{-3} , is an averaged mass of particles
108 with aerodynamic diameters of $100 \mu\text{m}$ or less collected from the air drawn through a filter in a
109 high-volume sampler over the sampling period of the test in proximity to the i -th stone quarry.
110 The testing was organized at a distance of (1-3) km from each quarry during the quarry' work.
111 Each test lasted 24 hours for collection of particles from about 2000 m^3 of air (EPA IO-2.1,
112 1999). The distribution of the test/measurement results c_{im} at the actual concentration c_i was
113 found to be normal with standard deviation equal to the standard measurement uncertainty $u_i =$

114 0.07 c_{im} and mean equal to c_i (Kuselman et al., 2012a). Corresponding likelihood functions are
 115 normal probability density functions (pdfs):

116

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

117

118 *2.1.2. Database and prior distributions of actual concentration values*

119

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

127

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

128

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

132

133 **2.2. Regulation and acceptance limits**

134

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

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

145

146 2.3. Particular risks of under- and overestimation

147

148 2.3.1. Particular specific risks

149

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

152

$$153 R_{ci(u)}^* = \int_{T_{Ui}}^{\infty} f(c_i|c_{im}) dc_i, \text{ for } c_{im} \leq T_{Ui}, \text{ and} \quad (5a)$$

154

$$155 R_{ci(o)}^* = \int_0^{T_{Ui}} f(c_i|c_{im}) dc_i, \text{ for } c_{im} > T_{Ui}, \quad (5b)$$

156

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

160

$$161 \quad f(c_i|c_{im}) = f(c_{im}|c_i)f(c_i) / \int_{-\infty}^{\infty} f(c_{im}|c_i)f(c_i) dc_i, \quad (5c)$$

162

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

164

165 2.3.2. Particular global risks

166

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

169

$$170 \quad R_{ci(u)} = \int_{T_{Ui}}^{\infty} \int_0^{T_{Ui}} f(c_{im}|c_i)f(c_i) dc_{im}dc_i, \quad (6a)$$

171

$$172 \quad R_{ci(o)} = \int_0^{T_{Ui}} \int_{T_{Ui}}^{\infty} f(c_{im}|c_i)f(c_i) dc_{im}dc_i. \quad (6b)$$

173

174 2.3.3. Probabilities of an acceptable test result and a conforming actual concentration value

175

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

179

$$180 \quad P(C_i) = \int_0^\infty \int_0^{T_{Ui}} f(c_{im}|c_i)f(c_i) dc_{im}dc_i . \quad (7a)$$

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

$$185 \quad P(\bar{B}_i) = \int_0^{T_{Ui}} f(c_i) dc_i . \quad (7b)$$

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 $P(\bar{C}) = 1 - P(C) = 1 - \prod_{i=1}^n P(C_i)$.

220

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

225 concentrations of all pollutants in this compartment conform to their regulation limits ($\bar{B} = \bar{B}_1 \cap$
 226 $\bar{B}_2 \cap \bar{B}_3$), whereas one or more test/measurement results c_{1m} , c_{2m} and c_{3m} exceed their
 227 acceptance limits. This event can occur when:

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

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

235 c) All the three measurement results exceed their acceptance limits. The total risk is
 236 $R_{\text{total(o)}}^* = P(\bar{B} | c_{1m}, c_{2m}, c_{3m}) = P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 | c_{1m}, c_{2m}, c_{3m})$.

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

239

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

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

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

243

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

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

247

248 $R_{\text{total(o)}}^* = \prod_{i=1}^{\nu} R_{ci(o)}^*$ (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 ν from all n pollutants under control.

252 From eqn (9) it follows that any one of ν 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 ν 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 (Pendrill 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.

271

272 *3.1.3. Total global risk*

273

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

277

$$278 R_{ci(o)} = P(\bar{B}_i \cap \bar{C}_i). \quad (10)$$

279

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

$$283 R_{total(o)} = P(\bar{B} \cap \bar{C}), \text{ where}$$

284

$$285 \bar{B} \cap \bar{C} = \bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap (\bar{C}_1 \cup \bar{C}_2 \cup \bar{C}_3) = (\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1) \cup (\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_2) \cup (\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_3). \quad (11)$$

287

288 The total global risk of overestimation is thus:

289

$$290 R_{total(o)} = P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1) + P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_2) + P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_3) - P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1 \cap \bar{C}_2) - P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1 \cap \bar{C}_3) - P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_2 \cap \bar{C}_3) + P(\bar{B}_1 \cap \bar{B}_2 \cap \bar{B}_3 \cap \bar{C}_1 \cap \bar{C}_2 \cap \bar{C}_3). \quad (12)$$

293

294 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 $\bar{B}_1 \cap \bar{C}_1$,
 295 $\bar{B}_2 \cap \bar{C}_2$ and $\bar{B}_3 \cap \bar{C}_3$ are also independent and equation (12) can be rewritten using notation (10)
 296 in the following way:

297

$$298 \quad R_{\text{total}(o)} =$$

$$299 \quad P(\bar{B}_2)P(\bar{B}_3)R_{c1(o)} + P(\bar{B}_1)P(\bar{B}_3)R_{c2(o)} + P(\bar{B}_1)P(\bar{B}_2)R_{c3(o)} - P(\bar{B}_3)R_{c1(o)}R_{c2(o)} -$$

$$300 \quad P(\bar{B}_2)R_{c1(o)}R_{c3(o)} - P(\bar{B}_1)R_{c2(o)}R_{c3(o)} + R_{c1(o)}R_{c2(o)}R_{c3(o)}. \quad (13)$$

301

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

304 In general, for any number n of pollutants

305

$$306 \quad R_{\text{total}(o)} =$$

$$307 \quad \sum_{i=1}^n (\prod_{l \neq i} P(\bar{B}_l)) R_{ci(o)} -$$

$$308 \quad \sum_{i=1}^n \sum_{j>i} (\prod_{l \neq i,j} P(\bar{B}_l)) (\prod_{q=i,j} R_{cq(o)}) +$$

$$309 \quad \sum_{i=1}^n \sum_{j>i} \sum_{k>j} (\prod_{l \neq i,j,k} P(\bar{B}_l)) (\prod_{q=i,j,k} R_{cq(o)}) + \dots + (-1)^{n-2} \sum_{i=1}^n P(\bar{B}_i) (\prod_{q \neq i} R_{cq(o)}) +$$

$$310 \quad (-1)^{n-1} \prod_{q=1}^n R_{cq(o)}, \quad (14)$$

311

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

313

314 3.2. Calculation

315

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

321 Core code developed in R programming environment for calculation of the risks is reported in
322 Annex A. Calculation of total specific risks of under- and overestimation by eqns (1) and (8),
323 respectively, using corresponding particular specific risk values by eqns (5), is shown in Section
324 A-1. Time spent for calculation of the total specific risks with a regular PC (Intel® Core™ i5-
325 3470 Processor, CPU @ 3.20 GHz, Windows 7 Professional 64 bit) is about one second. While
326 increasing (doubling, for example) the number of the involved components does not affect the
327 calculation time, decreasing the numerical integration parameter (stepsize) from 0.001 to 0.0001,
328 increases the execution time up to 6 seconds.

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

336

337 **4. Results and discussion**

338

339 4.1. Total specific risks of under- and overestimation

340

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

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

348 A case when only the second and the third quarries are active, is represented in Fig. 2b, where
 349 the total risk, $R_{total(u)}^*$, shown as a surface, depends on both c_{2m} and c_{3m} in the range $[0.010,$
 350 $0.200] \text{ mg m}^{-3}$. The surface lies mostly on the bottom of the three-dimensional region where
 351 $R_{total(u)}^*$ is close to zero, as in Fig. 2a, increasing with c_{2m} and c_{3m} approaching their tolerance
 352 limits $T_{U1} = T_{U2} = 0.200 \text{ mg m}^{-3}$. When both c_{2m} and c_{3m} simultaneously approach 0.200 mg m^{-3} ,
 353 this leads to a ‘protuberance’ in the total risk surface.

354 The same dependence of $R_{total(u)}^*$ on c_{2m} and c_{3m} is observed when all the three quarries are
 355 active simultaneously, but $c_{1m} < 0.170 \text{ mg m}^{-3}$: the contribution of the particular risk $R_{c1(u)}^*$ to the
 356 total one in such a case is negligible as shown in Fig. 2a. For comparison, Fig. 2c illustrates a
 357 scenario when all the three quarries are active and $R_{total(u)}^*$ - the surface - is depending on c_{2m}
 358 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
 359 seems very similar to Fig. 2b. However, the color scales of the $R_{total(u)}^*$ surfaces are different,
 360 since the scale in Fig. 2c is greater because of the significant contribution of $R_{c1(u)}^* = 0.211$ at
 361 $c_{1m} = 0.194 \text{ mg m}^{-3}$ (indicated in Fig 2a by dotted lines).

362 Dependence of the total specific risks of overestimation of the actual TSPM concentration in

Fig. 3 air on measurement results, when they are out-of-specification ($c_{im} > T_{Ui}$), is detailed in Fig. 3.

364 A case when only the first quarry is active, and the total risk $R_{\text{total(o)}}^*$ is equal to the particular

365 risk $R_{c1(o)}^*$, is shown in Fig. 3a by solid line 1. Dotted lines 3 and 2 point a measured TSPM

366 concentration $c_{1m} = 0.250 \text{ mg m}^{-3}$ and corresponding risk value $R_{c1(o)}^* = 0.008$, as an example.

367 Naturally, the risk of overestimation increases as c_{1m} approaches 0.200 mg m^{-3} (the tolerance

368 limit), and is close to zero for $c_{1m} > 0.260 \text{ mg m}^{-3}$.

369 The case when only the second and the third quarries are active, as in Fig 2b, and $R_{\text{total(o)}}^*$

370 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

371 maximum $R_{\text{total(o)}}^*$ value is observed as c_{2m} and c_{3m} near the tolerance limit simultaneously.

372 Fig. 3c illustrates a case when all the three quarries are active, as in Fig. 2c, but $c_{1m} = 0.250$

373 mg m^{-3} . The scale of the $R_{\text{total(u)}}^*$ surface, shown by the color bar, is two orders less than in Fig.

374 3b. The reason is that the total risk of overestimation, defined as a product of the three particular

375 risks, is influenced by the contribution of $R_{c1(o)}^* = 0.008$ at $c_{1m} = 0.250 \text{ mg m}^{-3}$ (indicated in Fig

376 3a by dotted lines). In other words, if an out-of-specification measurement result is significantly

377 greater than the tolerance limit, the probability of violation of the regulation is high and the

378 particular risk of overestimation is low. Therefore the total specific risk of overestimation is low

379 also.

380

381 4.2. Total global risks of under- and overestimation

382

383 The particular global risks of underestimation $R_{c1(u)} = 0.006$, $R_{c2(u)} = 0.010$ and $R_{c3(u)} =$

384 0.005 obtained here are equal to the values published earlier (Kuselman et al., 2012a). They are

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

389 The particular global risks of overestimation are $R_{c1(o)} = 0.007$, $R_{c2(o)} = 0.015$ and $R_{c3(o)} =$
390 0.006 . They are also equal to those published by Kuselman et al. (2012a). The probabilities of
391 conforming actual concentration values calculated are $P(\bar{B}_1) = 0.951$, $P(\bar{B}_2) = 0.934$ and
392 $P(\bar{B}_3) = 0.965$. The total risk of overestimation, evaluated in the present work for the first time
393 as well, is $R_{\text{total}(o)} = 0.026$, again greater than each $R_{ci(o)}$.

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

397

398 5. Conclusions

399

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

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

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

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

415

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417

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419 Chemistry (IUPAC Project 2016-007-1-500).

420

421 **Appendix A. Core of the R code**

422

423 **A-1. Calculation of the total specific risks**

424

```
425 #####  
426 # Specific risks #  
427 #####  
428  
429 # Input data for the quarries  
430 mu1 = -2.326      # Prior location parameter for Q1  
431 mu2 = -2.031      # Prior location parameter for Q2  
432 mu3 = -2.338      # Prior location parameter for Q3  
433 sigma1 = 0.434    # Prior scale parameter for Q1  
434 sigma2 = 0.280    # Prior scale parameter for Q2  
435 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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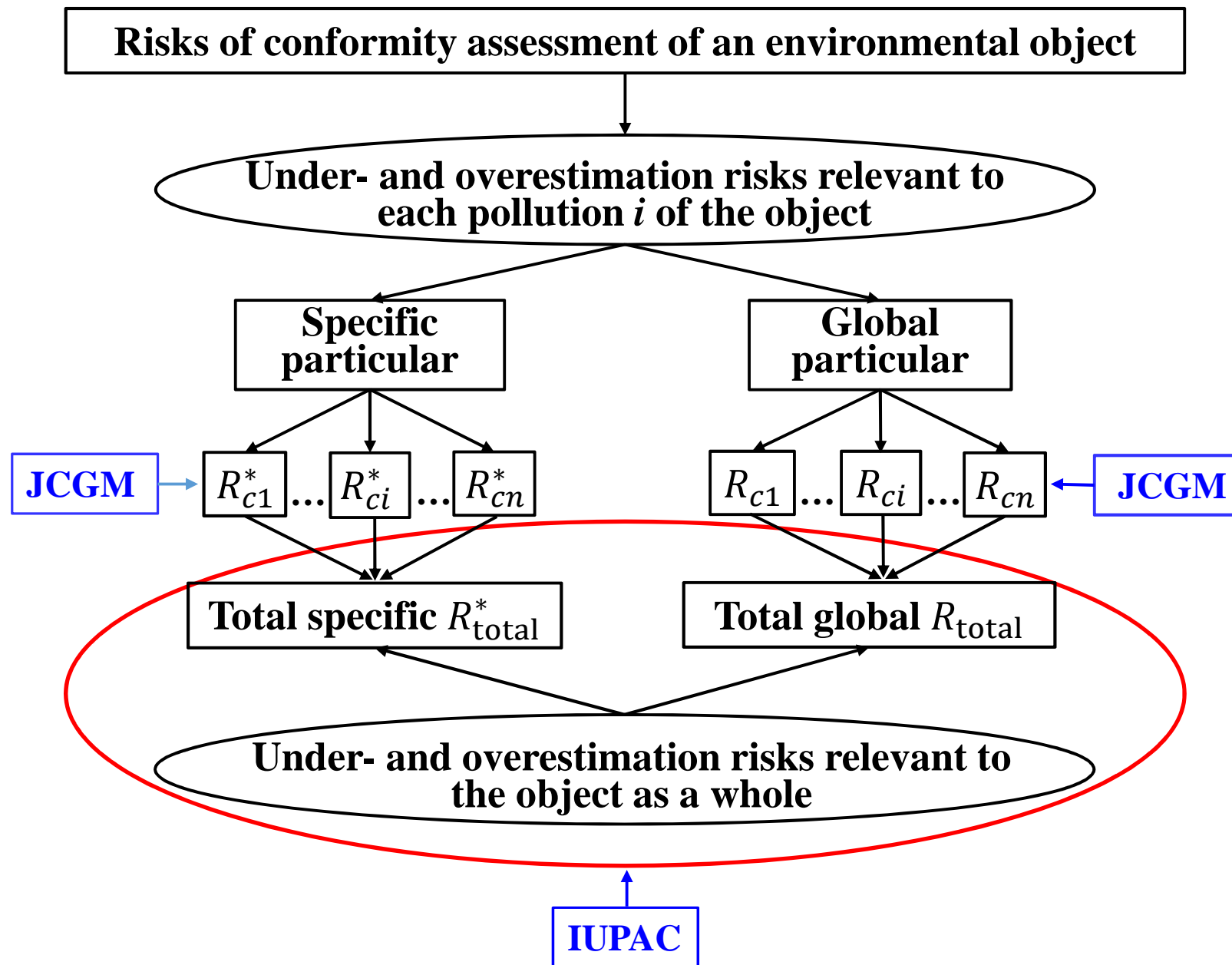
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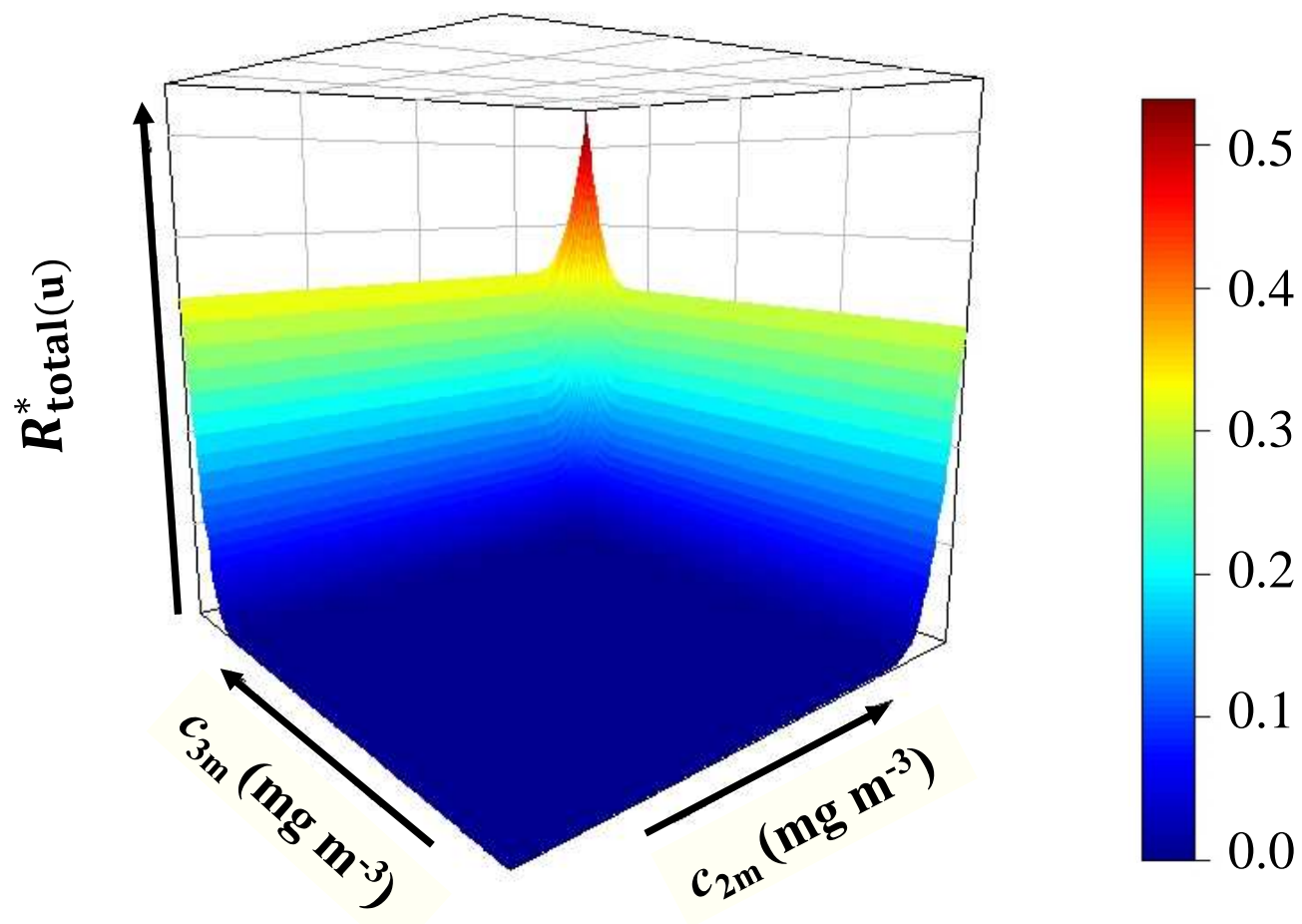
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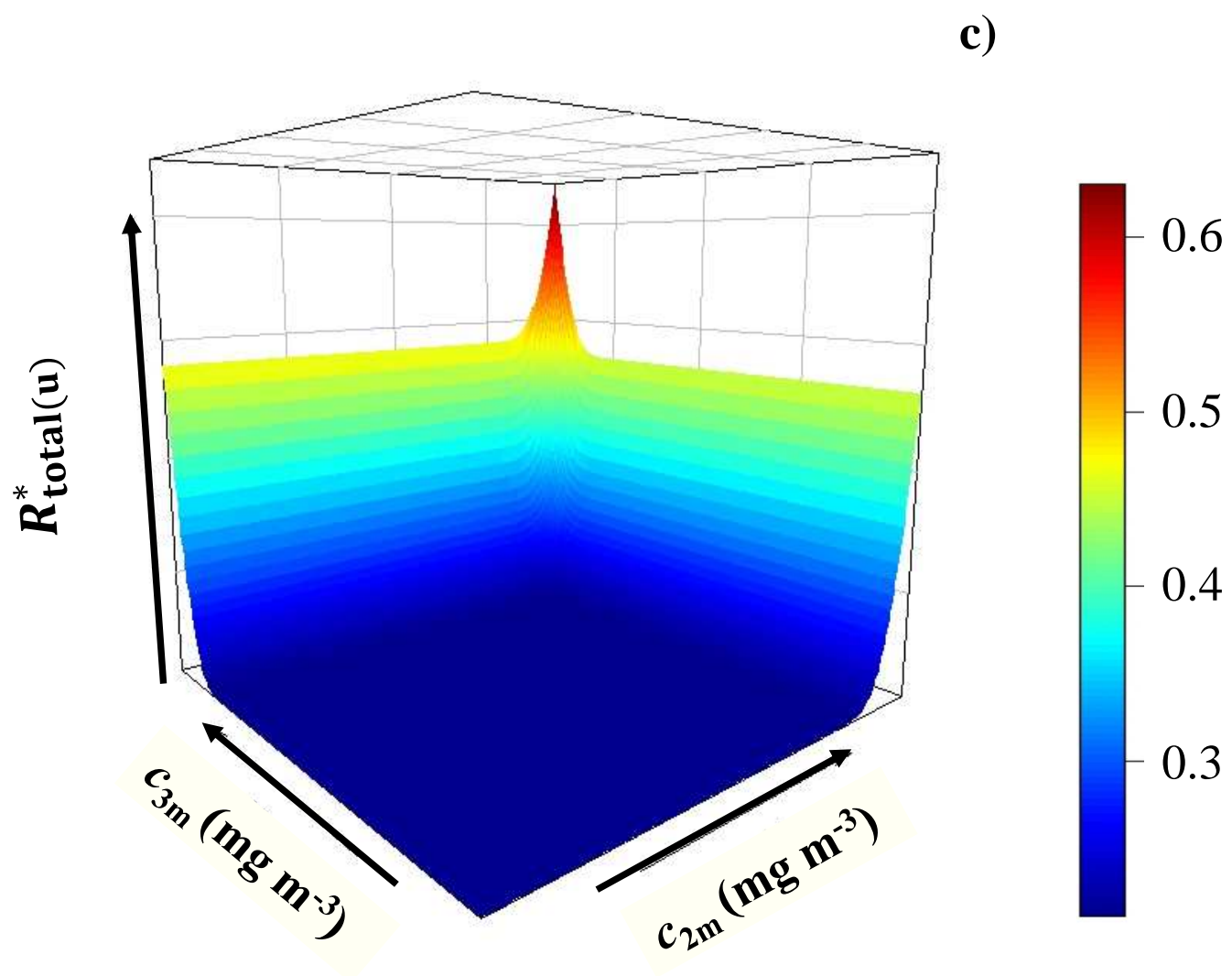
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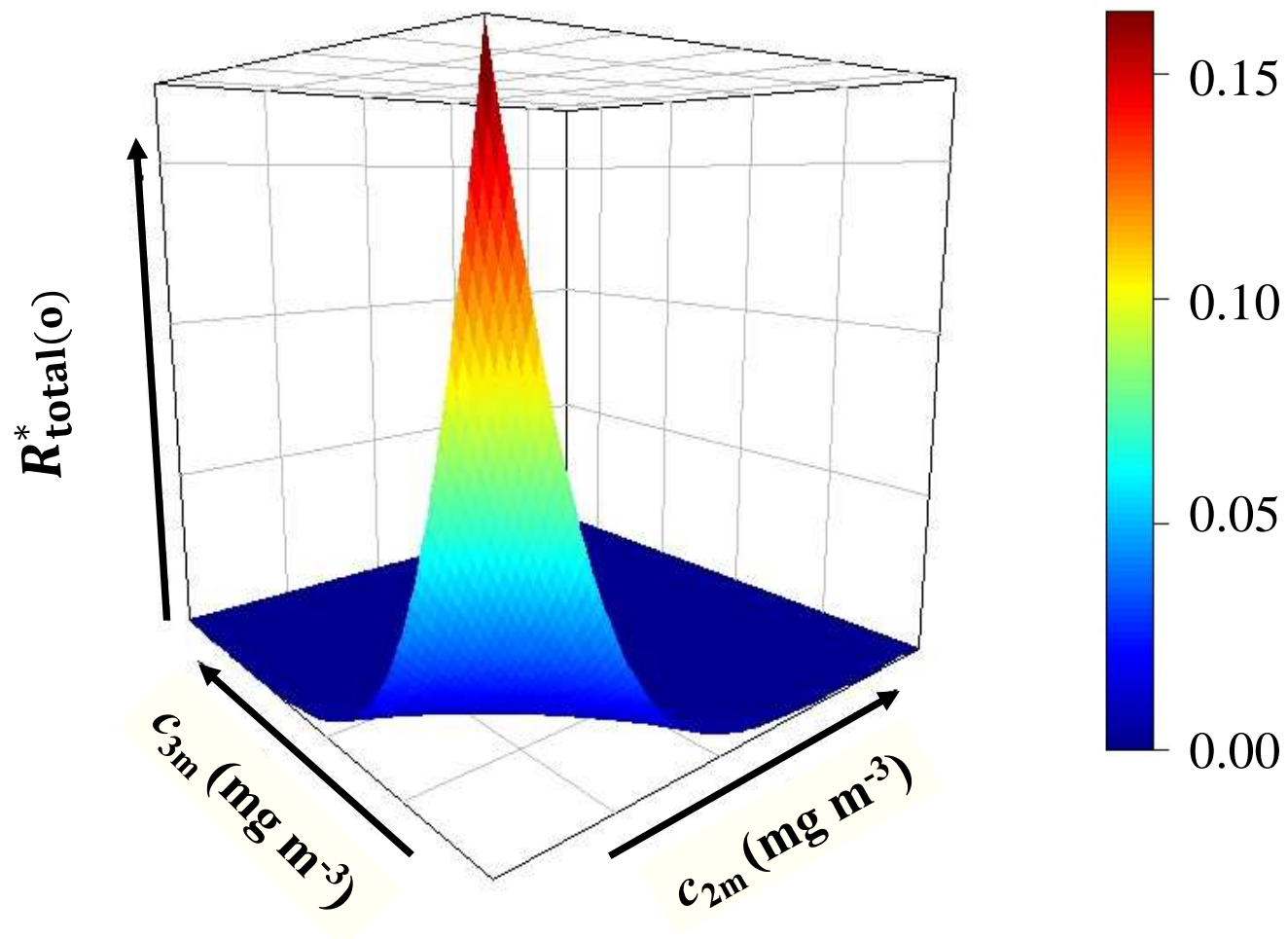


b)

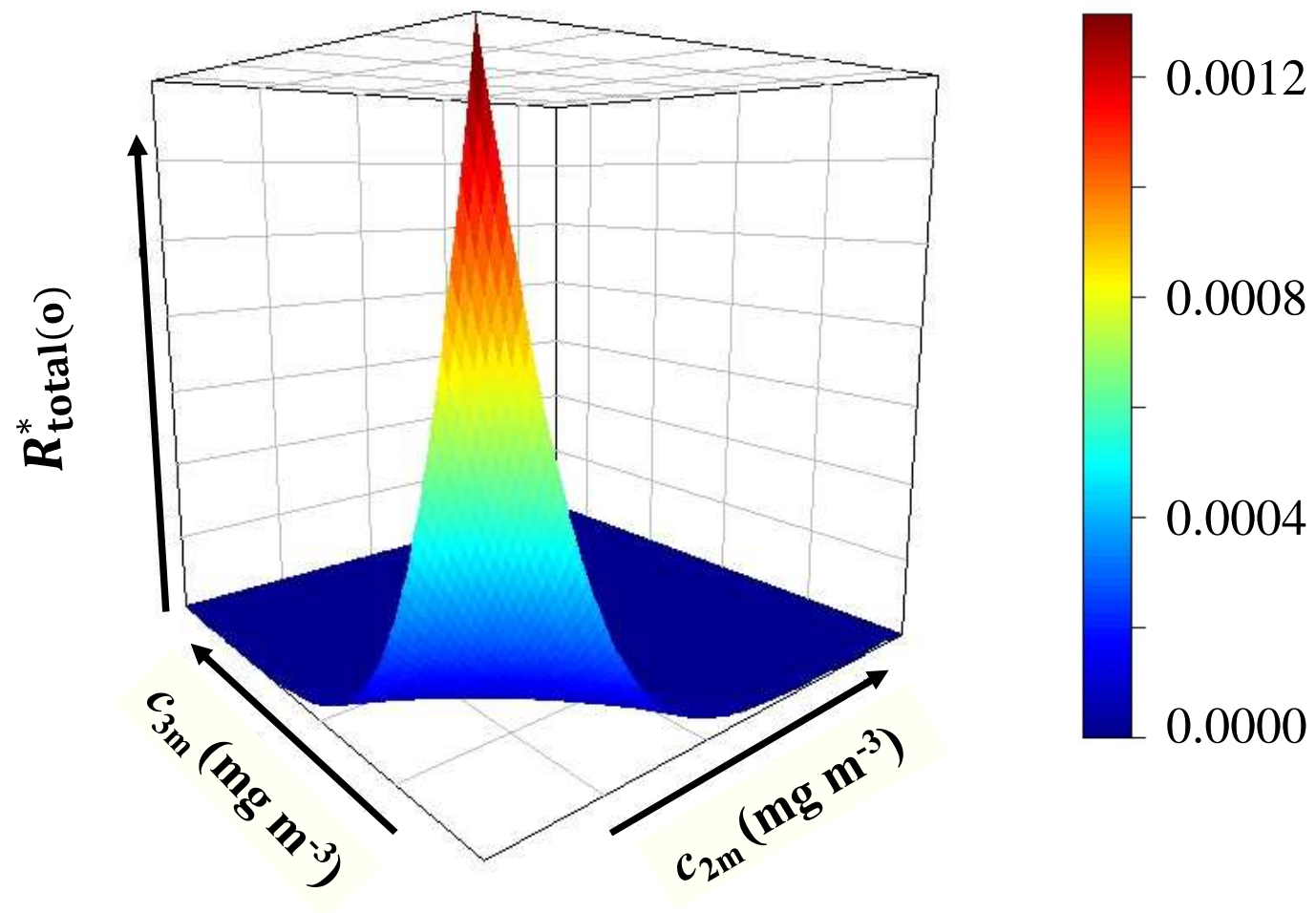


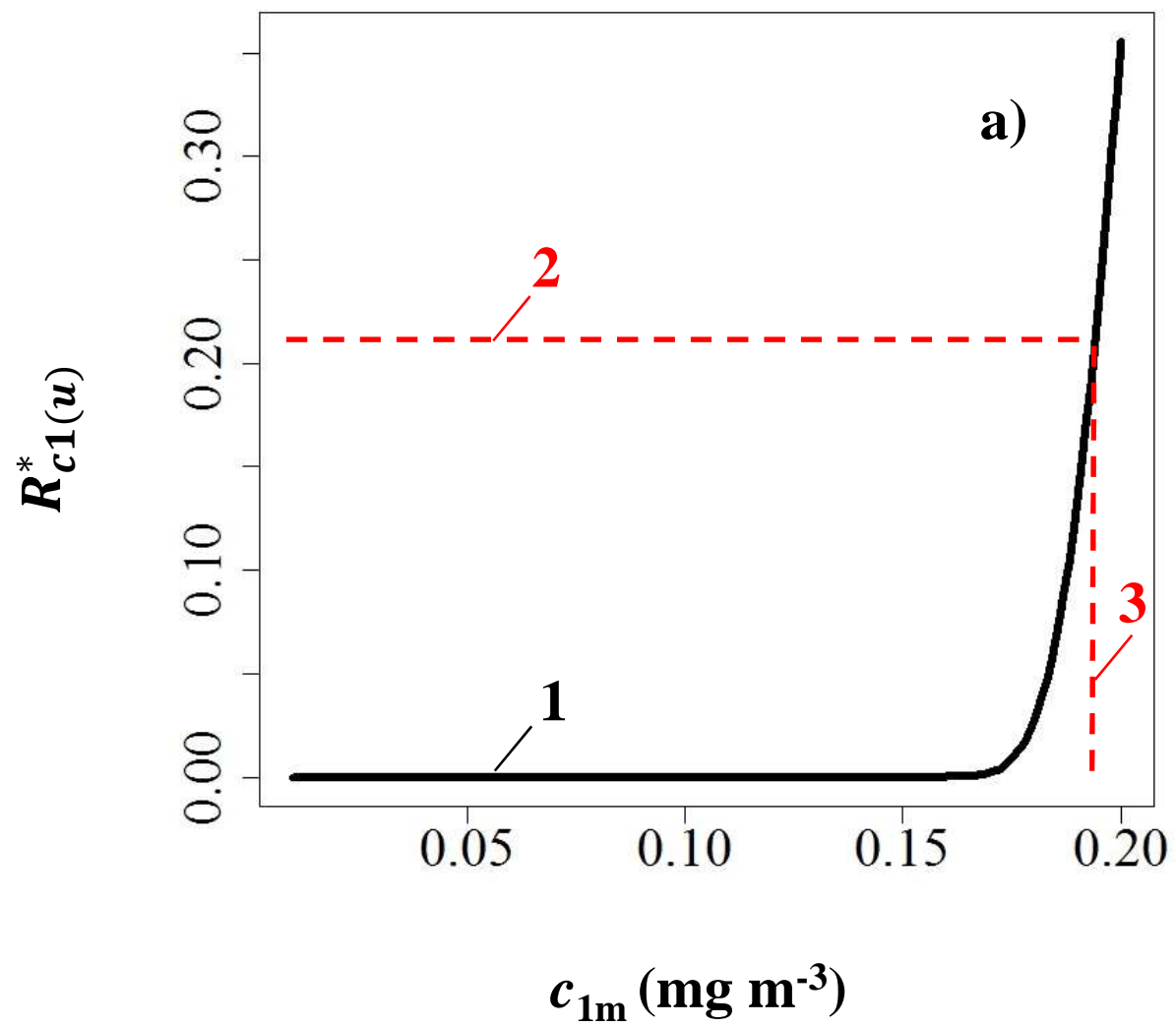


b)



c)





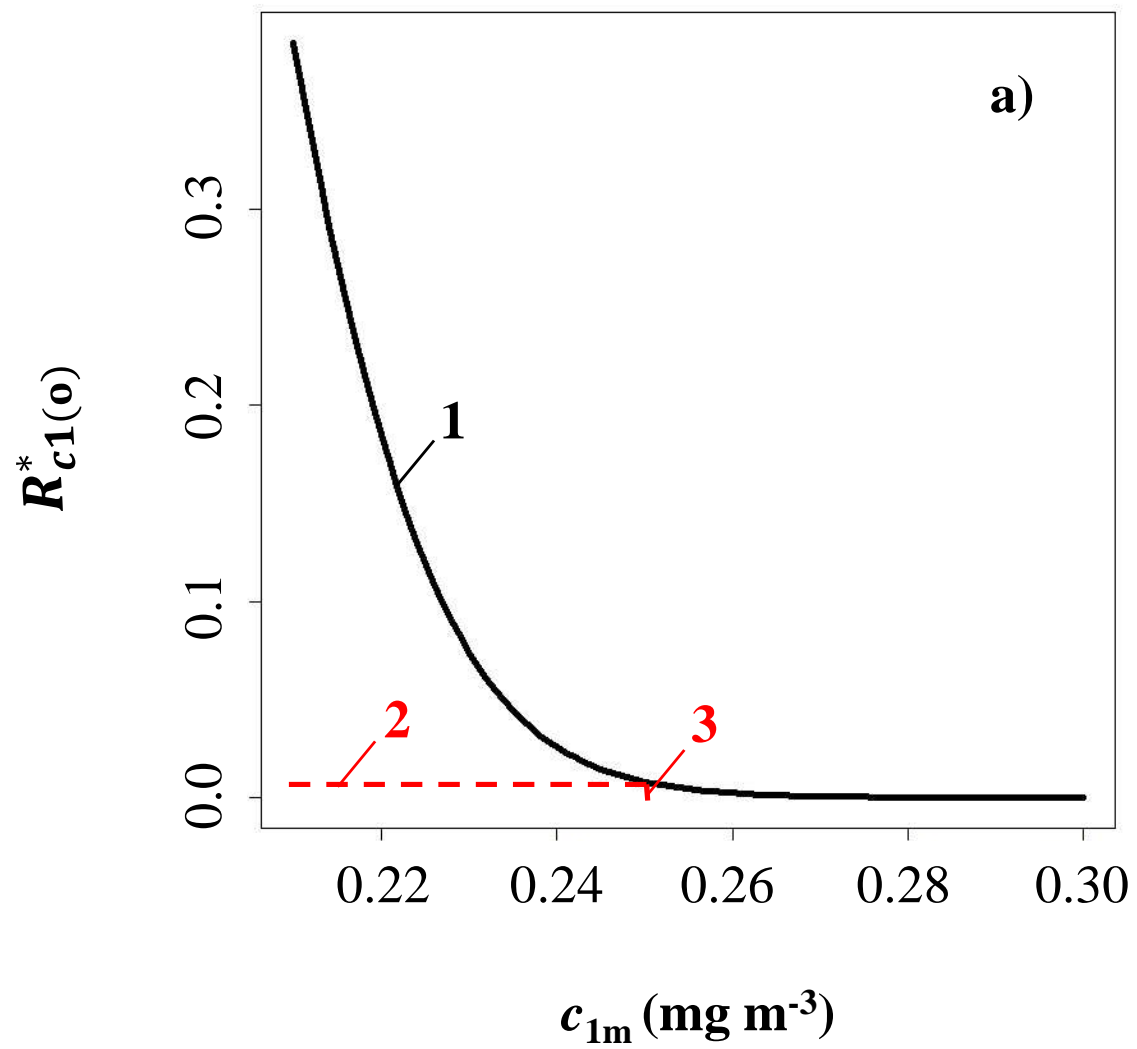


Figure captions

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_{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.