Conformity assessment of mass concentration of total suspended particulate matter in air

F. Pennecchi[1], F. Rolle[1], A. Allard[2], and S.L.R Ellison[3]

[1]INRIM, Istituto Nazionale di Ricerca Metrologica, Strada delle Cacce 91, 10135 Torino, Italy

[2]LNE, Laboratoire National de Métrologie et d'Essais, 29 avenue Roger Hennequin, 78197 Trappes Cedex, France

[3]LGC, Laboratory of the Government Chemist, Queens Road, Teddington, TW11 0LY, UK

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1 Summary

The main goal of the present study is to show how to calculate risks of false decisions in the conformity assessment of test results, according to the framework of [1], in the case in which a normal distribution is not a valid assumption for modelling prior information on the measurand. As a case study, test results of mass concentration of Total Suspended Particulate Matter (TSPM) in ambient air are considered.

2 Introduction of the application

A total of 496 test results of mass concentration of TSPM in ambient air, collected in 2009 in the proximity of three stone quarries located in Israel, were obtained according to the Environmental Protection Agency (EPA) method IO-2.1 [2]. Such results were compared with the national (Israeli) regulation limit for air quality to study the occurrence of Out-Of-Specification (OOS) test results, as detailed in [3] and in [4].

In the present example, the focus is on the calculation of global and specific risks of false decision in the conformity assessment of such kind of test results. The risk of underestimating the pollutant concentration is the consumer's/inhabitants' risk and that of overestimating is the producer's risk. Calculation of such risks is as important for the Regulator (the Ministry of Environmental Protection) protecting the inhabitants' quality of life in the area surrounding the quarries, as for the Manufacturers' Association acting in the interests of the stone producers in the country.

Risk values of false decisions on conformity of the TSPM concentration are here calculated for each quarry separately. Nonetheless, total risks of false decisions concerning the environmental compartment as a whole can also be calculated, hence characterizing the conformity of the TSPM concentration in the overall region encompassing the three quarries. Such total risks were modelled on the basis of the law of total probability in [5], but are out of the scope of the present example.

3 Specification of the measurand

For characterization of TSPM, the EPA method IO-2.1 [2] indicates the use of a high-volume sampler for collection of particles with aerodynamic diameters of 100 µm or less. A large volume V of air, in the range $1\,600\,\mathrm{m}^3$ to $2\,400\,\mathrm{m}^3$, was typically sampled at an average rate and the mass m of the matter in the sampled air volume, collected on the sampler filter, was measured as the difference between the results of weighing the filter before and after sampling. The measurand is the average value of the TSPM mass concentration over the sampling period: $c = m/V$ $(\mathrm{mg\,m^{-3}})$. In this study, TSPM from the i-th quarry, $i = 1, 2, 3$, is considered as the i-th pollutant.

4 Test results and associated measurement uncertainty

Three quarries were monitored by the Israeli National Physics Laboratory (INPL) at four points in the compass approximately 1 km to 3 km from each quarry, four to five times per month. A total of 496 test results were collected (220 relevant to quarry 1, 176 to quarry 2 and 100 to quarry 3), each test lasting 24 h. In [3] it was demonstrated, by means of the analysis of variance (ANOVA), that the monthly variation was not a significant factor in the data variability, whereas TSPM mass concentration seemed significantly influenced by the factor 'quarry'. Thus, it was concluded that the anthropogenic contributions to TSPM mass concentration due to the activity of the quarries were dominant and the test results for each quarry had to be studied separately.

Measured TSPM concentration values c_m are reported (in $\mathrm{mg\,m^{-3}}$) within Q1data.txt, Q2data and Q3data.txt files for quarry 1, 2 and 3, respectively (available in the repository [6]), and depicted in figure 1.

A full uncertainty budget for the considered test results is available in [3], where it was shown that the major contribution to the combined measurement uncertainty associated with the results is that coming from the measurement of the sampled air volume. The combined relative standard uncertainty associated with a typical test result was evaluated as 7.0 %. No correlation among test results from different quarries was observed.

5 Tolerance limits

The Israeli national regulations of ambient air quality prescribe an upper tolerance (regulation) limit $T_\mathrm{U} = 0.2\,\mathrm{mg\,m^{-3}}$ for TSPM mass concentration for 24 h sampling. This limit holds for any location, also close to the quarry. Hence, for each quarry and at any sampling point, $T_{\mathrm{U}i} = 0.2\,\mathrm{mg\,m^{-3}}$, for $i = 1, 2, 3$.

6 Decision rule and conformity assessment

Regulations require direct comparison of measured values $c_{i\mathrm{m}}$ with $T_{\mathrm{U}i}$. In the present example, acceptance limits $A_{\mathrm{U}i}$ will be made varying in order to show their impact on the risk values of false decisions. When acceptance limits are taken to coincide with the tolerance limits (that is, $A_{\mathrm{U}i} = T_{\mathrm{U}i}$), a "shared risk" rule is considered as the decision rule for conformity assessment [1, sec. 8.2.1].

In the present example, the consumers are the inhabitants living in the area surrounding the quarries, whereas the producers are the owners of the stone quarries.

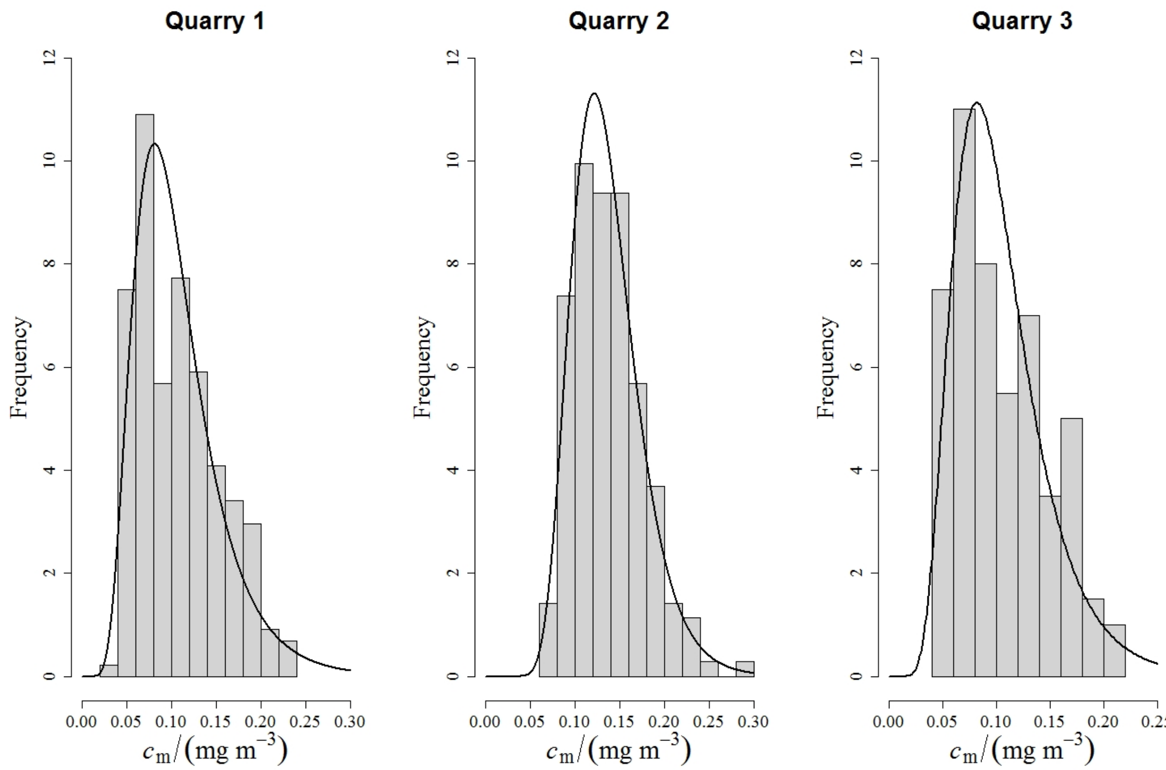

Figure 1: Histograms of the measured TSPM mass concentration values for each quarry and corresponding lognormal probability density functions smoothing the data.

The global and specific risks of false decisions in conformity assessment are defined in [1, sec. 3.3] for both the consumer and the producer, and have different interpretations. While a specific risk is the risk of an incorrect decision made for a particular measurement result, global risks refer to the probability of an incorrect decision based on a future measurement. Both kinds of risks rely on a Bayesian framework but require the calculation of different probability objects. Indeed, the posterior distribution (obtained through Bayes' theorem) is used for specific risks while the joint distribution is used for global risks.

6.1 Bayesian framework

In the framework of the JCGM document on the role of measurement uncertainty in conformity assessment, the evaluation of risks of false decisions on a characteristic of an item is described in [1, clause 9.3.2 and 9.5.2] for specific and global risks, respectively.

The underlying Bayesian approach requires defining a prior probability density function (PDF) $g_0(c_i)$ for the "true" values of TSPM mass concentration. Based on the Kolmogorov–Smirnov criterion of goodness-of-fit, the widely-used null hypothesis of a normal PDF was tested on the data available for each quarry and had to be rejected [3]. The normal distribution was found instead to be the best-fitting distribution for the experimental results after their logarithmic transformation. Therefore, for each quarry i, a lognormal distribution was chosen for modelling the actual values of TSPM mass concentration c_i:

$$g_0(c_i) = \frac{1}{c_i \sigma_i \sqrt{2\pi}} \exp\left[-\frac{(\ln(c_i) - \mu_i)^2}{2\sigma_i^2}\right], \tag{1}$$

whose distributional parameters are reported (on the logarithmic scale) in table 1. They were taken respectively as the mean and the standard deviation of the log-transformed data. The corresponding lognormal prior PDFs are the curves approximating the histograms in figure 1.

Table 1: Location and scale parameters of the prior PDF for each quarry.

Quarry i	Location parameter μ_i (adimensional)	Scale parameter σ_i (adimensional)
1	−2.325	0.434
2	−2.031	0.279
3	−2.337	0.402

The distribution of the measurement results $c_{i\mathrm{m}}$ at an actual concentration c_i was modelled by a normal distribution with expectation equal to c_i and standard deviation equal to the standard measurement uncertainty $u_i = 0.07 c_{i\mathrm{m}}$ [3]. The corresponding likelihood for each quarry is hence a normal PDF:

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

When both the prior PDF and the likelihood are normal distributions, the posterior PDF [1, Eq. (1)] is also normal [1, Sec. 7.2.1][1]. In such a case, the evaluation of specific and global risks is straightforward, as detailed in [1] . In the present example, instead, the prior PDF is lognormal, for each quarry, hence requiring some numerical approximation of the consumer's and producer's risks.

6.2 Global risks

For each quarry, and for any considered (upper) acceptance limit A_U, global risks for the consumer and the producer were calculated as a numerical approximation of the (double) integral of the product of the prior PDF (1) and the likelihood (2), according to [1, equations (19) and (20)]. In the considered case, since all the involved PDFs were defined on the positive axis only, the lower integration limits (both T_L and U_L) were taken as zero. Details of the calculation are in the code file A123_Global_risk_TSPM.r (available in the repository [6]), where the .r function dlnorm was used for evaluating the density of the considered lognormal distributions, whose logarithms have the mean and the standard deviation, reported in table 1 for each quarry, of the data distributions on the log scale (note that the log-transformed data have a normal distribution by the definition of the lognormal distribution). The integration of the joint PDF was performed by means of the R function `integrate`.

The obtained consumer's (red line) and producer's (blue line) global risks are displayed in figure 2, for A_U values varying in the interval $[T_\mathrm{U} - 0.05, T_\mathrm{U} + 0.05]$ mg m^{-3}. Considering, for example, the special case in which $A_\mathrm{U} = T_\mathrm{U}$, consumer's and producer's global risks were respectively 0.58 %

[1] If the prior information is meagre and the likelihood function is characterised by a normal distribution, then the posterior PDF is approximately normal [1, Sec. 7.2.2].

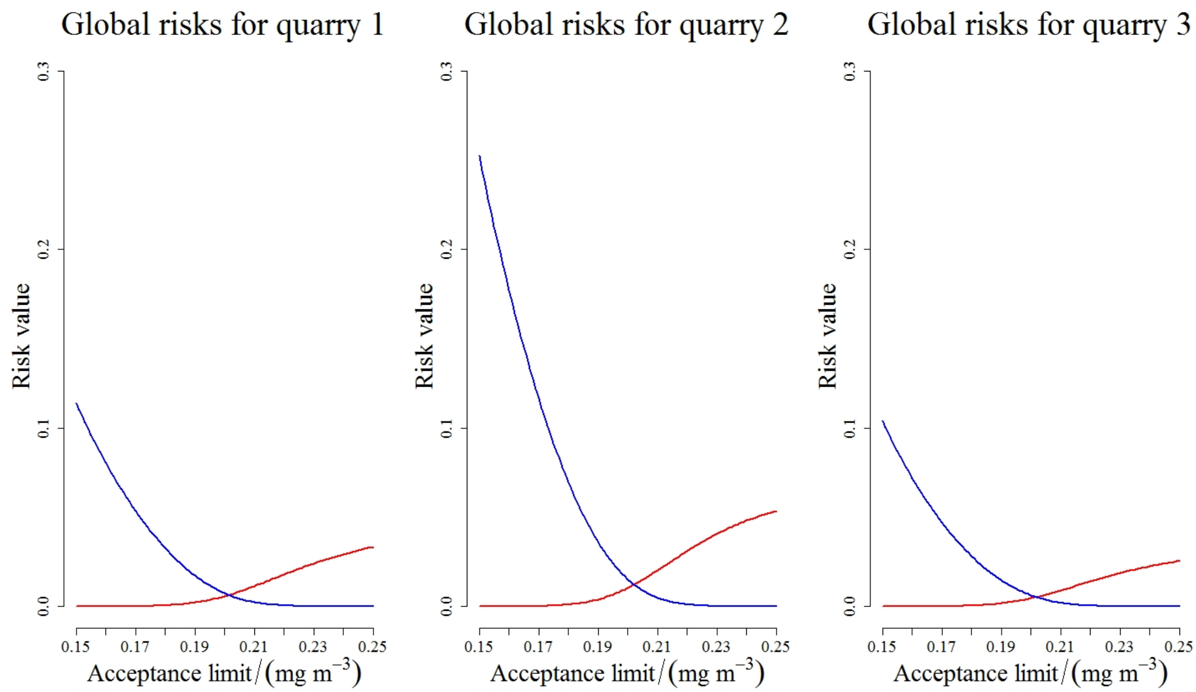

Figure 2: Consumer's (red line) and producer's (blue line) global risks versus acceptance limit values.

and 0.74 % for quarry 1, 1.04 % and 1.52 % for quarry 2, and 0.46 % and 0.62 % for quarry 3. Focusing on quarry 1, for example, one could be interested in finding the maximum acceptable A_{U} in order to have a desired small consumer's risk, let us say 0.01 %: it turns out that such an acceptance limit should not exceed 0.17 mg m^{-3}. However, in this case, the global producer's risk would increase from 0.74 % to about 5 %. The other way round, A_{U} should be at least equal to 0.23 mg m^{-3} in order to assure a producer's risk smaller than 0.01 %, again. In this case, the global consumer's risk would increase from 0.58 % to about 2 %.

6.3 Specific risks

For each quarry i, and just for the special case $A_{\mathrm{U}} = T_{\mathrm{U}}$, specific risks for the consumer and the producer were calculated according to the framework of [1, Sec. 9.3.2]. For a specific value $c_{im} < A_{\mathrm{U}}$ (that is, the measured TSPM mass concentration is assessed as conforming to the regulation limit), the consumer's specific risk is the integral of the posterior PDF $h(c_i|c_{im})$ on the region $[T_{\mathrm{U}}, \infty]$, that is on the region of true values which would not be actually conforming. For a specific value $c_{im} > A_{\mathrm{U}}$ (that is, the test result is not conforming to the regulation limit), the producer's specific risk is the integral of the posterior PDF on the region $[0, T_{\mathrm{U}}]$, the region of actually conforming true values. In both cases, the posterior PDF $h(c_i|c_{im})$ [1, equation A.11] was needed, but in the considered case it does not have a closed form because the prior PDF is lognormal.

Details of the calculation are in the code file A123_Specific_risk_TSPM.r (available in the repository [6]), where, for each c_{im} value, the posterior PDF was evaluated as the exponential of the log-posterior PDF, the latter being implemented as the sum of the log-prior PDF, evaluated in c_i, and the corresponding log-likelihood function at c_{im} (i.e., the logarithm of a normal PDF, with mean c_i and standard deviation equal to $0.07\,c_{im}$, evaluated at c_{im}). The integral of the posterior PDF was calculated by means of the R function `integrate`.

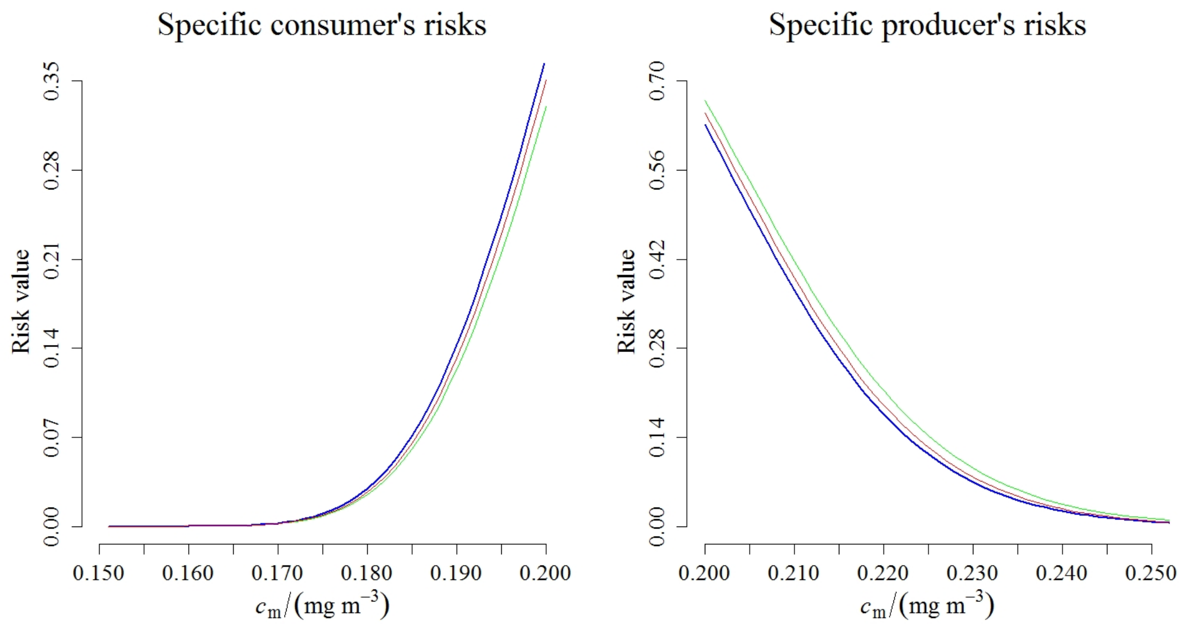

Figure 3: Consumer's and producer's specific risks versus test results, for quarry 1 (blue line), 2 (green line) and 3 (red line).

The obtained consumer's and producer's specific risks are displayed in Figure 3 (when $A_U = T_U$) for quarry 1 – blue line, quarry 2 – green line and quarry 3 – red line. They are plotted versus values c_{im} varying in the interval $[0.15, T_U]$ mg m^{-3} and $[T_U, 0.25]$ mg m^{-3} for the consumer and the producer, respectively.

These results have been validated against those from CASoft [7], which relies on simulation using a Metropolis-Hastings algorithm to estimate the posterior distribution used to calculate the specific risks. The results agreed within the small random variation expected for Monte Carlo estimates of small probabilities.

7 Interpretation of results

Studies on global risks, such as that conducted in section 6.2, can allow the involved parties (consumers and producers) to agree on an acceptance limit (balancing the safeguarding of the inhabitants' health and the economical interests of the quarries' owners, in the considered example).

The approach in section 6.3 provides risks of false decision for a specific test result and for a particular acceptance limit ($A_U = T_U$, in the considered case). From a practical point of view, no action will be undertaken when a measurement result is under the acceptance limit, that is when it is conforming with the requirements. However, when a test result exceeds the limit, it will be declared as non conforming and some corrective action will be required. In this case, the producer has at hand a tool for assessing the extent of his/her responsibility for such failure and possibly elaborate an appropriate reaction. As an example, for a non-conforming test result $c_{1m} = 0.225$ mg m^{-3}, the specific producer's risk for quarry 1 is about 12 %, meaning that there is a non-negligible 12 %

probability of such a test result to correspond to an actually conforming true value c_1.

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