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[Not translated]

Ambient air - Methodology for the assessment of the performance of source apportionment modelling system applications

Außenluft - Methodik zur Erfassung der Leistungsfähigkeit von Systemanwendungen zur Quellenzuordnung

Air ambiant - Méthodologie d'évaluation des performances dapplications de modélisation de l'attribution des sources et des récepteurs

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This draft Technical Specification is submitted to CEN members for Vote. It has been drawn up by the Technical Committee CEN/TC 264.

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EUROPEAN COMMITTEE FOR STANDARDIZATION
COMITÉ EUROPÉEN DE NORMALISATION
EUROPÄISCHES KOMITEE FÜR NORMUNG

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European foreword

This document (FprCEN/TS 17458:2019) has been prepared by Technical Committee CEN/TC 264 “Air quality”, the secretariat of which is held by DIN.

This document is currently submitted to the vote.

1 Scope

The European Directive on ambient air quality and cleaner air for Europe (2008/50/EC; AQD) identifies different uses for modelling: Assessment, planning, forecast and source apportionment (SA). This document addresses source apportionment modelling and specifies performance tests to check whether given criteria for receptor oriented source apportionment models (RM) are met. The scope of the tests set out in this document is the performance assessment of SA of particulate matter using RM in the context of the European Directives 2004/107/EC and AQD, including the Commission Implementing Decision 2011/850/EU of 12 December 2011. The application of RM does not quantify the spatial origin of particulate matter; hence, this document does not test spatial SA.

This document addresses RM users: practitioners of individual source apportionment studies as well as participants and organizers of source apportionment intercomparison studies. This document is suitable for the evaluation of results of a specific SA modelling system with respect to reference values (a priori known or calculated on the basis of intercomparison participants' values) in the following application areas:

— Assessment of performance and uncertainties of a modelling system or modelling system set up using the indicators laid down in this document.

— Testing and comparing different source apportionment outputs in a specific situation (applying an evaluation data set) using the indicators laid down in this document.

— QA/QC tests every time practitioners run a modelling system.

It should be noted for clarity that the procedures and calculations presented in this document cannot be used to check the performance of a specific SA modelling result without having any a priori reference information about the contributions of sources/source categories.

NOTE The application of this document implies that the intercomparison is organized and coordinated by an institution with the necessary technical capabilities and independence; the definition of which is beyond the scope of this document.

The principles of RM are summarized in Annex A. An overview of uncertainty sources and recommendations about steps to follow in SA studies are provided in Annex B and Annex C. For further information about SA methodologies, refer to e.g. [1; 2; 3].

There are methodologies different from RM which are widely used to accomplish SA, e.g. source oriented models. These other methodologies cover aspects of SA which are required in the AQD and are not addressed by RM (e.g. allocation of pollutants to geographic emission areas). Performance assessment of such methodologies is out of the scope of this document.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 13528:2015, *Statistical methods for use in proficiency testing by interlaboratory comparison*

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

3.1
candidate modelling system
modelling system or modelling system set up that is being tested in the intercomparison or being applied in isolation

3.2
candidate source
every source or source category present in the result of a SA candidate modelling system which is tested with the methodology described in this document

3.3
coordinator
organisation with responsibility for coordinating all activities involved in the operation of an intercomparison exercise

3.4
contribution-to-species
mass of each single chemical element or compound forming part of a (composite) pollutant apportioned to a source or source category, expressed as a percentage

Note 1 to entry: Depending on the type of SA modelling applications, this concept could be referred to as: "contribution by species" in CMB 8.2, "explained variation" in PMF 2, "percentage of species total matrix" in EPA PMF v3, and "factor fingerprint" in EPA-PMF v5.

3.5
input uncertainty
statistical dispersion of the values that can be reasonably attributed to every single species ambient concentration in the input matrix of receptor oriented models

3.6
derived source profile
relative chemical composition of the source or source category, resulting from a SA model run, expressed as parts per unit mass of every chemical species with respect to the total source or source category mass

3.7
factor
underlying latent variable identified by a multivariate analysis SA model (e.g. factor analysis or singular value decomposition) associated with an air pollution source or source category

3.8
maximum accepted distance
maximum Euclidean distance, on a cartesian plane, between the point representing the values (concentration ratios) of a chemical species in two source profiles, one on the abscissa and the other on the ordinate, and the identity line, which is considered acceptable to indicate the similarity of the two values

3.9
output uncertainty
uncertainty attributed to the average source contribution estimate (SCE), expressed in the same units, for a given time window of a source or source category in a source apportionment application result

3.10
receptor oriented models
models that, using as input the measured concentrations of pollutants at a given site (receptor) in a defined time window, provide source contribution estimates (SCEs) by applying multivariate analysis

3.11
reference source profile
source profile used as reference for the similarity tests of derived source profiles. In general, the reference source profiles are chemical profiles obtained from samples collected specifically to characterise the source or source category and which are available in the literature or in public repositories (e.g. SPECIATE, SPECIEUROPE)

3.12
reference value
a priori known or calculated source contribution estimate (SCE) attributed to a source or source category, represented by an evaluation dataset

3.13
results
output obtained by running a candidate modelling system using an evaluation dataset. The source apportionment results consist of e.g.: source contribution estimates (SCEs) including their output uncertainty, derived source profiles, source contribution time series and contribution-to-species

3.14
source apportionment (SA)
practice of deriving quantitative information about the contribution of sources and/or source categories to the concentration of pollutants at a given point or area in a defined time window

3.15
source category
group of air pollution sources of the same type that are characterised by similar chemical composition and/or temporal profile

3.16
source contribution estimate (SCE)
amount of the pollutant expressed as mass concentration (e.g. μg m^{-3}), attributed to a specific source or source category in SA model application results

3.17
source of air pollution
any human activity or natural process that causes pollutants to be released into the atmosphere or to be produced in the atmosphere

3.18
source profile
relative chemical composition of a (composite) pollutant emitted from an air pollution source expressed as the ratio of the mass of every single chemical species to the total mass of the pollutant

3.19
source oriented models
models that, starting from emission inventories, meteorological fields and boundary conditions, simulate the physical and/or chemical atmospheric processes affecting the emitted pollutants

3.20
species
single chemical elements or compounds that compose the studied pollutant when it is a family of compounds or an aggregate (composite)

3.21
pollutant
collective term meaning the total mass of the substance for which source contribution estimates (SCEs) are determined using source apportionment methods

Note 1 to entry: It could either be a single chemical compound (e.g. Hg), a family of similar chemical compounds (e.g. polycyclic aromatic hydrocarbons) or composite: an aggregation of different chemical compounds (e.g. particulate matter).

4 Symbols and abbreviations

fr tests	found-reference tests
ff tests	found-found tests
M_t	sum of the SCEs of all the candidate sources k in time step t of a given result
M	sum of the time averaged SCEs of all the candidate sources k of a given result
O_t	observed mass concentration of the pollutant in time step t
O	time averaged observed mass concentration of the pollutant
Pearson	Pearson product-moment correlation coefficient (r_{xy})
RM	receptor oriented source apportionment model
$RMSE_u$	uncertainty normalized root mean square error
$RMSE_{\sigma_o}$	root mean square error weighted by the standard deviation of the observations
r_{xy}	Pearson product-moment correlation coefficient (Pearson)
SA	source apportionment
SCE	source contribution estimate (mass concentration)
SID	standardized identity distance
WD	weighted distance
x_{kt}	SCE of candidate source k in time step t
x_k	average SCE of candidate source k
X_{kt}	reference value for the SCE of source k in time step t
X_k	reference value for the average SCE of source k
u_{Xkt}	standard uncertainty of X_{kt}
u_{Xk}	standard uncertainty of X_k

z	z-score
σ_p	uncertainty for proficiency test
ζ	zeta-score

5 Fundamentals of the evaluation methodology

The goal of the procedures and tests described in this document is to assess the performance of receptor oriented SA modelling applications. This is done by comparing the results of the tested SA candidate modelling system using as input pre-defined evaluation data sets with the reference values for the used data set (details in 7.1 and 7.2).

The evaluation methodology applied to the SA results encompasses three types of tests: complementary tests, similarity tests and performance tests. The similarity and performance tests are carried out independently for every candidate source or source category reported in the results. Hereon, the term "source" includes both source and source category, unless explicitly mentioned.

The complementary tests provide ancillary information about the overall consistency of the SA results. They do not assess the accuracy of the factor/source contributions' identification and quantification. The complementary tests include a) the apportioned pollutant mass test, consisting of the comparison between the pollutant reference mass (e.g. gravimetric mass) and the sum of the SCEs of all the sources and b) the comparison among the number of sources in every reported SA result or, if available, with the reference number of sources (see 8.1).

NOTE For the purposes of this document, the following SCEs are considered: a) the values for every sample or time step and b) their average for the entire time window represented by the evaluation data set.

The similarity tests assess whether a candidate source in a SA result obtained with a candidate modelling system can be allocated to a source category. The outcome of these tests is used to select the candidates for the determination of the reference values (see 7.2.1). To that end, the candidate sources are compared with reference source profiles (fr tests). In the absence of reference source profiles, all the candidate sources attributed to a source category are compared among each other (ff tests). The similarity tests compare the sources based on their chemical profiles, the time series of their SCEs, and their contribution-to-species. When provided, the uncertainty of the derived source profiles in the reported results is tested by comparison with the uncertainty of the reference source profiles (see 8.2 on similarity indicators).

The performance of a candidate SA modelling system is evaluated by comparing the SCEs of the candidate sources, resulting from runs with a given evaluation data set, with the reference values for that specific data set. The outcome of the performance test depends on whether the difference between the candidate and the reference meets a pre-established quality objective (see 8.3).

There are two types of performance tests: a) tests based on the z-scores (ISO 13528:2015), for the average SCEs of the time window represented in the evaluation data set (x_k) and b) tests based on the uncertainty normalized root mean square error ($RMSE_u$) [4; 5] for the time series of the SCEs (x_{kt}).

Candidates passing the z-score test are considered to have an average SCE for the entire modelled period comparable with the reference value. Candidates passing the $RMSE_u$ test are considered to have a SCE time trend for the modelled period comparable with the reference value. Candidates passing both tests have a performance which is considered "sufficient" for the purposes of the present document.

6 Arrays of tests

The tests to apply vary according to the objective of the application: individual run or intercomparison exercise.

In the individual runs a practitioner executes a source apportionment application using as input a data set for which the SCE reference values are not available. The array of tests for individual runs is reported in Annex D.

In intercomparison exercises, more practitioners execute SA models using as input the same evaluation data set (see 7.1) and the SCE reference values (*X*) are either available in advance (SA applications using synthetic evaluation data sets) or are calculated from the participant results. SA applications using synthetic evaluation data sets are included in this category. The array of tests for intercomparison exercises are reported in Annex E.

7 The performance assessment method

7.1 Evaluation data sets

The evaluation data sets used as input for the candidate modelling systems are derived from observed data or are synthetic.

The evaluation data sets consist of a matrix with the concentrations of selected chemical species in the ambient air measured at a receptor site over a given time-window and with a given time-resolution. The input uncertainties of the entries in the matrix are provided. The principles for the development of state-of-the-art data sets to be used as input for RMs are described in [1]. Distributing additional information about the study site or area (e.g. measured source profiles, pollutant concentrations, meteorological data, etc.) is optional. Siting information about the monitoring location of the observed data shall be also distributed.

Synthetic evaluation data sets are created by fixing the contribution of sources in every sample or time step. The concentration of the chemical species in the synthetic evaluation data sets is mathematically coherent with the source contributions. To create synthetic evaluation data sets, noise is added using randomization techniques and attributing an input uncertainty to the entries of the evaluation data set proportional to the noise e.g. [6].

The result of the performance assessment described in this document is associated with the classification of the monitoring site location represented in the evaluation data set (e.g. urban background, regional background, sites close to one specific source) and, therefore, it is not providing evidence about the performance of the candidate modelling system for different site classifications.

NOTE Estimating the transferability of the performance assessment obtained with one evaluation data set to classes of sites not present in the evaluation data set is beyond the scope of this document.

7.2 Determination of the SCE reference values and their standard uncertainties

7.2.1 Consensus value from participants

When executing a SA model using real-world evaluation data sets, the true SCEs values are unknown. Therefore, for this kind of evaluation data set the results reported by participants in intercomparison exercises are used to calculate the reference values.

The reference values for the averaged SCE (X_k) and for the SCE in every time step (X_{kt}) and their standard uncertainties u_{Xk} and u_{Xkt} are calculated for every source (*k*) separately. Such reference values are associated with the evaluation data set of observations that was used as input for the intercomparison. The best estimators of the reference values and their uncertainties are the robust average and standard