CNR - National Research Council of Italy
Institute of Atmospheric Pollution Research

Progress in the CEN TC 264/ WG 44 on SA

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CEN/TC 264

25th plenary meeting of CEN/TC 264
27 and 28 May 2015
Rome, Italy

Decision 939 (Rome 12)

CEN/TC 264 decides to establish CEN/TC 264/WG 44 "Source apportionment" in order to elaborate prCEN/TS xxxxx *"Ambient air – Methodology for the assessment of the performance of source apportionment model applications".* The secretariat is kindly provided by DIN (secretary: Mr. Simon Jaeckel).

Progress in the CEN TC 264/ WG 44 on SA

European Commission

WG 44 members

1	Convenor	CEN/TC 264	-		Mr.	Belis, Claudio A.
2	Secretary	DIN	Germany		Mr.	Jäckel, Simon
3	Committee Member	AENOR (Expert)	Spain		Mr.	Alastuey Uros, Jose Andres
4	Committee Member	AENOR (Expert)	Spain		Mr.	AMATO, Fulvio
5	Committee Member	AENOR (Expert)	Spain		Ms.	Karanasiou, Angeliki
6	Committee Member	AENOR (Expert)	Spain		Ms.	Minguillon, Mari Cruz
7	Committee Member	AFNOR (Expert)	France		Mr.	Alleman, Laurent
8	Committee Member	AFNOR (Expert)	France		Mr.	Bessagnet, Bertrand
9	Committee Member	AFNOR (Expert)	France		Mr.	Duclaux, Olivier
10	Committee Member	AFNOR (Expert)	France		Mr.	Favez, Olivier
11	Committee Member	AFNOR (Expert)	France		Ms.	Lhuillery, Caroline
12	Committee Member	ASI (Expert)	Austria		Mr.	Skomorowski, Paul
13	Committee Member	BSI (Expert)	United Kingdom		Mr.	Brookes, Daniel
14	Committee Member	BSI (Expert)	United Kingdom		Mr.	Stedman, John
15	Committee Member	DIN (Expert)	Germany		Mr.	Müller, Wolfgang J.
16	Committee Member	DIN (Expert)	Germany		Mr.	Nordmann, Stephan
17	Committee Member	DIN (Expert)	Germany		Mr.	Quass, Ulrich
18	Committee Member	DS (Expert)	Denmark		Mr.	Olesen, Helge Rørdam
19	Committee Member	ECOS (Europe) (Expert)	-		Ms.	Blondeau, Marjolaine
20	Committee Member	ECOS (Europe) (Expert)	-		Mr.	Moorcroft, Stephen
21	Committee Member	NBN (Expert)	Belgium		Mr.	Bergmans, Benjamin
22	Committee Member	NBN (Expert)	Belgium		Mr.	Lenartz, Fabian
23	Committee Member	NEN (Expert)	Netherlands		Mr.	van Pul, Addo
24	Committee Member	NEN (Expert)	Netherlands		Mr.	Wesseling, Joost
25	Committee Member	SN (Expert)	Norway		Ms.	Guerreiro, Cristina
26	Committee Member	UNI (Expert)	Italy		Ms.	Pietrodangelo, Adriana
27	Document Monitor	ASI	Austria		Mr.	Nachbaur, Joerg
28	Document Monitor	NEN	Netherlands		Ms.	van Hoek, Caroline
29	Document Monitor	SIS	Sweden		Mr.	Yoler, Jimmy

18 →29 members
8 → 11 countries represented
+ ECOS
+ European Comm.

Belis CA

Joint Research Centre

CEN TC264 WG 44, Apr 2016

Connections with other initiatives

JRC initiative on Source Apportionment

FAIRMODE, mainly WG3

- ✓ Literature review (constantly update),
- ✓ Intercomparisons (2 finished 1 in progress),
- ✓ Drafting Guidances (first one published in 2014, review foreseen 2016/7)
- ✓ Development of a method for evaluating intercomparison
- ✓ Creation of databases: SPECIEUROPE, Database of world SA studies
- ✓ Training

AQUILA

- ✓ intercomparison (proficiency tests)
- ✓ evaluation of measurement uncertainty (GUM)
- ✓ test and development of analytical methods

IAEA, Regional Project on APM 1013 (2014-2015)

WHO, evaluation of health burden

Danube Air Nexus, Support EU strategy in the Danube area, 3 pilot areas

Belis C.A. CEN TC264 WG 44, Oct 2015

Technical Specification (CEN/TS)
"Ambient air — Methodology for the assessment of the performance of source apportionment modelling system applications"

Scope : to specify '***performance tests to meet given quality objectives for source apportionment modelling systems***', by statistical indicators laid down in the TS.

Pertinence : ***'…restricted to the assessment of source apportionment in the context of the European Air Quality Directive.'***

End-users : ***'organizers of intercomparison studies as well as practitioners of source apportionment studies'***

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Modelling systems:

receptor-oriented, RO, (CMB and MFA) and **source-oriented, SO,** (CTMs) models

Pollutants:

'…the following pollutants will be considered to be included in the scope of the CEN/TS:

PM10, PM2,5, BC (EC), VOC, organic aerosol (OA) and POPs for receptor models;

and **PM10, PM2,5, O3, NO2, BC (EC) and SO2** for source oriented models.'

Time resolution:

Annual, seasonal, daily, hourly

Application areas:

- *'assessment of performance and uncertainties of a modelling system…'*
- *'testing and comparing different source apportionment outputs in a specific situation (dataset)…'*
- *'QA/QC tests every time practitioners run a modelling system'.*

The TS *'…is not prescribing the methodology to accomplish the source apportionment.'*

WG 44 plans to include annex with suggestions on the best tools for SA.

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Preliminary list of TASKS that need further scientific work, in case research is being financed by EC in relation to a standardization mandate:

- receptor oriented versus source oriented models comparison;
- acceptability ranges for different pollutants should be derived from testing;
- selection of species (sensitivity test);
- estimation of rotational ambiguity;
- evaluation on metrics (e.g. SID vs. Pearson, weighted distance).

The list will be refined and further discussed at the next meeting.

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Evaluation methodology

Parameters and properties of the candidate modelling system are assessed by complementary, similarity and performance tests.

The CEN/TS specifies cases where each test has to be considered ***essential*** **(E)**, ***facultative*** **(F) or *not applicable* (N.A.)**, according to :
goal of the modelling (individual use by practitioners or intercomparison studies led by a coordinator), modelling parameter, test category, RO or SO model.

The CEN/TS also encompasses comparison between receptor-oriented and source-oriented models. However :

tests to compare RO vs SO modelling performances require further scientific work;
sensitivity tests (variation of input data; base case vs scenarios: only applicable to SO models) also need further discussion.

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Performance assessment method

The CEN/TS specifies requirements of the testing datasets to be used as input in the candidate modelling system:

For RO models: *'…matrix with the concentration of selected chemical species in the ambient air in a receptor over a given time-window. The input uncertainties of the entries in the matrix are provided. Additional information…'*

For SO models: '…*emission inventories, meteorological fields and boundary conditions for the modelled domain over the considered time window. Measurements at ground level monitoring stations may be also provided for modelling validation purposes.'*

Testing datasets for source-oriented models require further discussion to meet SO modellers needs

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Performance assessment method

The CEN/TS specifies requirements of the reference value and its standard uncertainty of testing datasets, for assessment purposes:

for testing datasets of observations:
a consensus value from participants is used, defined as
'…the assigned value and its standard uncertainty determined as the robust average and robust standard uncertainty (ISO 13528), respectively, of the results that pass the similarity tests.'

for testing datasets of synthetic data:
'…the reference value X and its uncertainty ux are known a priori.'

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Acceptability ranges of testing indicators

Complementary tests

Mass closure

- Analysis of the linear regression parameters
- RMSE

'SCEs averages (xi) falling within ±20% of the measured mass concentration are in general considered suitable…' for RO models

More discussion about ranges with FAIRMODE and CEN TC264/ WG43

Number of identified sources

distance from the median of histogram / reference: within ±3

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Similarity tests

'The sources that obtain acceptable scores in at least 50% of the similarity tests are considered comparable to the reference source.'

Chemical profile

- Pearson product-moment correlation coefficient: 0.6
- Standardized Identity Distance (SID): k parameter set for every source/source category
- Weighted Distance (WD) (model estimated uncertainty): within twice the combined uncertainty (WD=2)

Time series

- Pearson product-moment correlation coefficient: 0.6

Contribution-to-species (%)

- Pearson product-moment correlation coefficient: 0.6

Standardized Identity Distance (SID):

'The parameter k is the acceptability criterion for the distance between two species expressed as a fraction of the average of the mass of the species in the two profiles. Considering that sources have different degree of variability it is convenient to set k values for every source/source category….'

'A list of suggested k values to account for the chemical variability of the most common PM sources in the public repositories is available..' (Belis et al., 2015, AE).

$$SID_{xy} = \frac{1}{m}\sum_{j=1}^{m}\frac{ID_j}{MAD_j} = \frac{1}{m}\sum_{j}\frac{\frac{1}{\sqrt{2}}|x_j - y_j|}{k\,\frac{1}{2}|x_j + y_j|}$$

m is the number of species, ID is the identity distance, MAD is the maximum acceptance distance, xj and yj are the concentrations of the species j in the sources x and y

'Additional contributions to the k value can be attributed to the analytical uncertainty and to secondary pollutants..'

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Weighted Distance (WD):

bias of every species in the source profile scaled by its uncertainty and the one of the reference. Uncertainty estimated by models reflects the analytical uncertainty in most cases.

'Distances up to twice the combined uncertainty, corresponding to WD=2 are considered acceptable.'

$$WD_{xy} = \frac{1}{m}\sum_{j=1}^{m}\frac{|x_j - y_j|}{\sqrt{u_{xj}^2 + u_{yj}^2}}$$

ux_j and uy_j is the uncertainty of the concentration of species in the chemical profile of sources x and y respectively

Performance indicators :

Source Contribution Estimates (SCEs) from intercomparison studies

Average SCEs:

Z-score (ISO 13528) : *'…the quality objective is defined as the relative standard deviation for proficiency assessment (σp). This value is set to 50% by analogy with the data quality objectives for modelling uncertainty of the annual average of PM10 laid down in Directive 2008/50/EC.'*

$$z_{sce} = \frac{x_i - X}{\sigma_p}$$

x_i is the candidate SCE; σ_p is the relative standard deviation for proficiency assessment

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Performance indicators :

Source Contribution Estimates (SCEs) from intercomparison studies

Tme series of SCEs:

Normalised Root Mean Square Error (RMSEu) :

'The acceptability criterion is the condition where the model random error is equivalent or lower than twice the standard uncertainty of the reference (RMSEu ≤1).'

$$RMSE_u = \frac{\sqrt{\frac{1}{n}\sum_1^n (m_i - r_i)^2}}{2u}$$

(Thunis et al., 2012, AE)

m and r denote the modelled and reference values for the n observations and u the standard uncertainty of the reference SCE time series.

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SCEs model estimated uncertainty and method reproducibility :

- Interquartile range and the 2.5 – 97.5 percentile range of all the reported results

'The intercomparison exercise makes it possible to test the reproducibility of a method intended as the range of results reported by different practitioners using the same or similar tools.'

- Zeta-score (ISO 13528) :

'The zeta-scores of SA results have been observed to follow a normal distribution..' (Belis et al., 2015, AE), ***'therefore the critical values: -3, -2, 2 and 3 are proposed (ISO 13528).***

In order to assess participants' uncertainty estimation, zeta-scores should be used in conjunction with z-scores.

Sources with acceptable z-scores and poor zeta-scores likely have underestimated uncertainties.

$$\zeta_{sce} = \frac{x_i - X}{\sqrt{u_{xi}^2 + u_X^2}}$$

xi is the candidate SCE

WG44: further issues under discussion and TASKS

CEN/TS structure:

in the present form of the TS, no sharp indications are provided to include/exclude a solution. It seems to allow the coordinator of the IE deciding if leave a solution (factor profile/source contribution provided by each participant) or exclude it.

Requirements of testing datasets (section 6.1):

local agencies can be concerned about the amount of data that is given in this section as mandatory .

A solution could be to make available a package of datasets ready to be used for QA/QC of SA. On-line tool connected to SPECIEUROPE?

WG 44 agrees that if a tool for assessment of source apportionment results will be developed, this should be done in an open source environment (R) to ensure transparency. In case the Delta Tool will be used, the feasibility to translate this into R should be checked.

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WG44: further issues under discussion and TASKS

Sensitivity tests (SO models):
to be suggested as essential (E) or facultative (F)?

Rotational ambiguity (RO models):
the only output of RM actually not considered in the TS

Criticity of grouping of sources:
the coordinator of the intercomparison should have the option to group similar source contributions to improve comparability of solutions

Flow diagrams to be added for each test category?

List of definitions to be extended (e.g.'pollutant' vs 'species'; time series /time pattern /temporal profile;…)

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CEN WG 44 meetings:

1st : Düsseldorf, Germany (14 – 15 October 2015)

2nd : Kjeller (Oslo), Norway (20 – 21 April 2016)

Next meeting: Vienna, Austria (9 – 10 November 2016)

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