Individualization of a representative daily trend of pollutant concentrations as characteristic scenario to be simulated by mathematical models

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ABSTRACT

The paper presents a daily trend of pollutant concentrations, referred to as the "representative day", i.e. the day for which the overall sum of the mean-square differences between its concentration, averaged within each hour, and the concentrations for all other days at the same hour, is a minimum. The approach also allows the identification of the "least representative day" (the daily series that maximises the mean sum of squared residuals).The purpose of such typifying is that of outlining characteristic scenarios for a given period under investigation and than mathematical models make it possible to attempt simulations of a typical period trend, without the need to simulate all the days of the time interval covered by the typical period.

1. INTRODUCTION

Air quality standards are important tools for legislators and local authorities in the control of air pollution. In order to verify respect of air quality standards a combination of measurements and models are required.

The interpretation of phenomena governing air pollution diffusion presupposes a synthesis of information derived from temporal data series. The recording of air pollution concentration values involves the measurement of a large volume of data, giving rise to the need for a rapid method of summarising such information. Generally, automatic selectors and explicators are used; many of which are provided by statistics (Seinfeld and Pandis, 1998).

Currently, hourly concentration means are the most widespread method employed and represents the maximum desegregation with which pollution data are generally collected. It is often adopted in applications and allows the evaluation of average concentrations over long periods, such as a day, a season or a year. In addition hourly concentrations are used to define specific "typical" periods that may be of particular interest in the study of pollutant diffusion (for example, a typical working day, a typical holiday, a typical seasonal day etc.) (Tirabassi and Rizza, 1993). The purpose of such typifying is that of outlining characteristic scenarios for a given period under investigation. Mathematical models make it possible to attempt simulations of a typical period trend, without the need to simulate all the days of the time interval covered by the typical period.

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2. THE REPRESENTATIVE DAY

What we call a "representative day" is a 24 hour data set, actually recorded at a field station, which is characterised by the least differences with respect to all the 24 hour measurements of that station's temporal series: that is to say, the daily series whose sum of the squared differences over 24 hours turns out to be the smallest compared to all the other days of the period under consideration.

In mathematical notation, the least squares matrix is indicated by *A*:

$$A_{ij} = \sum_{k=1}^{24} \left(c_{ki} - c_{kj} \right)^2 \qquad i, j = 1, 2...N$$
 (1)

where *N* is the number of days in the time period for which the representative day is calculated and c_{ki} is the pollutant concentration of the *i*-th day at the *k*-th hour.

We adopt A_i to indicate the sum of all the squared residuals of the *i*-th line (or column, A_{ij} being a symmetrical matrix with all zeros in the diagonal):

$$A_i = \left(\sum_{j=1}^N A_{ij}\right) \tag{2}$$

The representative day (RD) is the one with the lowest sum, i.e. the *i*-th day where A_i is the smallest of the quantities obtained:

$$\min(A_i) \Rightarrow \mathsf{RD} \tag{3}$$

The purpose of such typifying is that of outlining characteristic scenarios for a given period under investigation and than mathematical models make it possible to attempt simulations of a typical period trend, without the need to simulate all the days of the time interval covered by the typical period.

The approach also allows the identification of the "least representative day" (LRD), that is the daily series that maximises the mean sum of squared residuals:

$$\max(A_i) \Rightarrow \mathsf{LRD} \tag{4}$$

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The least representative day identifies an anomalous situation of pollutant dispersion, often (although not always) characterised by maximum ground concentrations. The study of the meteorological and emission parameters relating to this day, will allow a preliminary interpretation of the phenomena which brought about the situation.

To compare the degree of representativity of the most or least representative days with that obtained for other time periods and/or in other measurement stations (also in complete different areas), a normalisation is required in order to make the day independent of the length of the measurement series, sampling period and characteristics of the area under study.

The "representativity" of a representative day can be quantified by introducing the following adimensional index:

$$DI = \frac{\sqrt{\sum_{i=1}^{N} \sum_{k=1}^{24} (\Gamma_k - c_{ik})^2}}{\sqrt{\sum_{i=1}^{N} \sum_{k=1}^{24} (\overline{c_k} - c_{ik})^2}}$$
(5)

where $\overline{c_k}$ is the mean hourly concentration at the k-th hour calculated over the period under consideration and Γ_k is the mean hourly concentration of the representative day at the k-th hour.

DI is an adimensional quantity (DI \ge 1), which is closer to unit the more the day RD is representative of the period in consideration.

The least representative day can also be normalised in the same way: one simply substitutes in equation (5) the hourly concentration of RD (Γ_k) with the least representative ones. In this case the value of DI will be greater than one, providing an indication of the low degree of representativity of the day obtained; the more DI is greater than 1, the more the least representative day is "anomalous", compared to the trend of RD.

The normalisation procedure described above presents two important features:

- independence from the size of the measured concentrations (if the concentrations are multiplied by a factor, the results of the normalisation do not change);
- ii) independence from the number of days (*N*) included in the time period considered (the quantities of the numerator and denominator of equation (5) are calculated over all the *N* days of the period under consideration).

3. EXAMPLE OF APPLICATION TO THE URBAN AREA OF BOLOGNA

In Tirabassi and Nassetti (1999) we applied the method to the industrial area of Ravenna which is situated on flat terrain, 10 Km from the sea. In this paper the method has been applied to the metropolitan area of Bologna.

Bologna is a metropolitan area with half million inhabitants. It is situated on the North part of Italy and on the South border of the flat Po Valley. The climate is basically continental and the entire area is subject to a series of weak local circulations, frequent inversion phenomena ensuing high relative humidity, particularly during extended periods of anticyclonic conditions. Usually, perturbations are of north-westerly origin.

In particular, we considered the hourly mean series of data of SO_2 , NO_2 , CO, O_3 and particulate, collected during one year in a station situated downtawn.

An example of the results is shown in figures 1 - 5 relating to particulate SO_2 , NO_2 , CO and O_3 , respectively. In table 1 the dates on which the most and least representative days occurred, are reported, while, table 2 provides the representativity index DI of the most and least representative days.

Tab. 1. Day of the year on which the most (RD) and least representative (LRD) days occurred.

	Part.	SO ₂	NO ₂	CO	O ₃
RD	4 Dec	12 Oct	24 Jan	12 Feb	9 Oct
LRD	21 Oct	11 Nov	5 May	11 Dec	22 Jul

Tab. 2. The representative index DI of the most (RD) and least representative (LRD) days.

	Part.	SO ₂	NO ₂	CO	O ₃
RD	1.040	1.013	1.069	1.042	1.020
LRD	2.908	4.197	2.904	3.781	3.804

4. CONCLUSIONS

The interpretation of the phenomena governing pollutant diffusion requires a synthesis of the information given by temporal data series.

The most representative day constitutes a simple and immediate method through which to characterise the hourly structure of daily trend.

The most representative day constitutes a simple and immediate method through which to characterise the hourly structure of daily trends. We have called the "representatve day", the one which minimises the sum of squared differences with respect to all the daily trends in a temporal series. The attention is focused on the "day as a unit", without losing, however, the particular hourly structure.

The special advantage of the representative day method derives from the fact that, being an actual day; it allows the identification of the date on which the representative trend occurred and, thus, a knowledge of the meteorological and emission parameters that characterised it. It can therefore be more easily and less expensive simulated with diffusion models.

The same approach also allows the identification of the least representative day, that is, the day on which an anomalous,

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nearly always critical situation occurred, compared to the average trend recorded for that period.

5. REFERENCES

- Seinfeld J.H. and Pandis S.N. (1988). *Atmospheric Chemistry And Physics*. John Wiley & Sons, New York.
- Tirabassi T. and Rizza U. (1993). Flux Parameterization For Atmospheric-Diffusion Models In An industrialized area. *Il Nuovo Cimento*, 16 C, 187-192.
- Tirabassi T. E Nassetti S. (1999). The Rapresentative Day. *Atmos. Environ.*, 33, 2427-2434.



Fig. 1. Representative day (black circles), least representative day (black diamonds) and typical day (white squares) of particulate.



Fig. 2. Representative day (black circles), least representative day (black diamonds) and typical day (white squares) of SO₂



Fig. 3. Representative day (black circles), least representative day (black diamonds) and typical day (white squares) of NO₂



Fig. 4. Representative day (black circles), least representative day (black diamonds) and typical day (white squares) of CO



Fig. 5. Representative day (black circles), least representative day (black diamonds) and typical day (white squares) of O_3

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