Available online at www.sciencedirect.com
ScienceDirect
Atmospheric Environment 41 (2007) 9146–9158
ATMOSPHERIC ENVIRONMENT
www.elsevier.com/locate/atmosenv

Improvement of receptor model use in analytical aspect

Chu-Fang Wang[a], Pen-Chi Chiang[b], Man-Ting Cheng[c], Hung-Lung Chiang[d,*]

[a]*Department of Biomedical Engineering and Environmental Science, National Tsing-Hwa University, Hsinchu 30013, Taiwan*
[b]*Graduate Institute of Environmental Engineering, National Taiwan University, Taipei 10617, Taiwan*
[c]*Department of Environmental Engineering, National Chung-Hsing University, Taichung 402, Taiwan*
[d]*Department of Health Risk Management, China Medical University, Taichung 40402, Taiwan*

Received 10 April 2007; received in revised form 24 July 2007; accepted 30 July 2007

Abstract

In this study, four certified particle standards including NIST SRM 1648 urban particulate matter, BCR Reference Material No. 176 city waste incineration ash, NIST SRM 2709 San Joaquin soil, and NIST SRM 1633b coal fly ash were used to simulate ambient particulate matter. Twenty-five samples were prepared with the four certified particulate standards. A total of 23 elements were analyzed per sample, 19 by ICP-AES and ICP-MS, three by IC, and one element, Si, by spectrophotometer. Results showed that combining the three IC-analyzed ionic species with the 19 ICP-AES/MS analyzed elements into the CMB model did not improve the source identification significantly. In addition, when all 23 analyzed chemical species per sample were used in the CMB model, they were still not good enough to effectively make the parameters of the CMB model fit the statistical criteria. Some of high variation and low recovery chemical species, i.e. Cd, V, Sb, etc., may have caused poor CMB model simulation. Omitting some poor quality analyzed species (such as relative analysis error $>20\%$) could improve the CMB model simulation. Therefore, high quality chemical species data are important for the CMB model. In addition, co-linearity of source profiles also affects the CMB model; combining the co-linear sources could enhance the solubility of the CMB model. In this study, a two-step procedure was developed for CMB model simulation to improve source identification.

Keywords: Chemical mass balance (CMB); Receptor model; Fingerprints

1. Introduction

Since it was first proposed in the early 1970s (Hidy and Friedlander, 1972; Kneip et al., 1972; Winchester and Nifong, 1971), the chemical mass balance (CMB) receptor model has become one of the most successful mathematical methods used to apportion potential source contributions and to develop appropriate air quality management strategies (Gordon, 1980, 1988; Hopke and Dattner, 1982, 1985; Watson, 1989; Begum et al., 2005; Kim et al., 2005; Marmur et al., 2005; Ward and Smith, 2005; Feng et al., 2006). However, one of the largest impediments to the receptor model today is the lack of accurate, precise, and comparable analytical data for determining chemical profiles (''fingerprints'') of ambient and source data sets (Wang et al., 1995a, b; Robinson et al., 2006; Bhave et al., 2007).

The chemical composition of ambient air samples is by no means needed quantitatively as input for

*Corresponding author. Tel.: +886 4 2207 9685; fax: +886 4 2207 9687.
E-mail address: hlchiang@mail.cmu.edu.tw (H.-L. Chiang).

1352-2310/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.atmosenv.2007.07.052

the CMB receptor model. The obtained analytical data contain not only direct information on the concentrations measured during each sampling period, but also a wealth of indirect information in the correlations that exist between the pollution sources and sampling sites (Gordon, 1980). The CMB model input data include the ambient concentrations of various species and their fractional amount in each source-type emission. However, even with the best of sampling and analytical methods, only a limited number of species are generally available for the subsequent model analysis. Thus, in a complex air shed, the resolution and precision of the model analysis may not only be limited by the number of chemical species but also by the reliability of these data on which the mathematical analysis is based. To obtain a better CMB result the uncertainty estimates of these values are required. It is therefore necessary to weigh the importance of input data values in the solution and to calculate the uncertainties of the source contributions. Currently used CMB software (Watson et al., 1990, 1998; Christensen, 2004; Christensen and Gunst, 2004) applies the effective variance solution which can provide realistic estimates of the uncertainties for the source contributions and give greater influence to chemical species with higher precision in both the source and receptor measurements than to species with lower precision.

The CMB model assumptions include constant compositions of source emissions, no reaction between chemical species, known characterized information about emission sources, linearly independent of source compositions and enough chemical information about the species. These assumptions for the CMB model are fairly restrictive and difficult to comply with in actual practice. A number of tests to determine the CMB model's abilities to tolerate deviations from these assumptions have been performed (Gordon et al., 1981; Henry, 1982; Currie et al., 1984; Dzubay et al., 1984; DeCesar et al., 1985; Javitz et al., 1988a, b; Christensen and Gunst, 2004). All these tests obtained the same conclusions that deviations from these assumptions increase the stated uncertainties of the source contribution estimates. None of them has ever quantified the influence of accurate and precise chemical information on the estimated source contributions.

This paper evaluates the influence of obtained analytical data on the solution of source contributions via the CMB model analysis and presents a two-step data evaluation procedure for evaluating the precision of analytical data of CMB modeling instead of optimizing analytical data. To provide sufficient information on air samples in an effort to improve the resolution of receptor model analysis, an experiment using mixed standards to simulate real samples and test the model analysis has been performed.

2. Materials and methods

2.1. Selection of source profiles

To verify the effectiveness of the CMB model from the extent of the number of chemical species and the precision and accuracy of chemical species in samples, four standard sources was selected to simulate the particulate sources in ambient air: (1) NIST SRM 1648 urban particulate matter, (2) BCR Reference Material No. 176 city waste incineration ash, (3) NIST SRM 2709 San Joaquin soil, and (4) NIST SRM 1633b coal fly ash. Among these simulated sources, waste incineration ash and coal fly ash can be categorized as industrial-type "smoke-stacks" and are considered area sources in emission inventories. On the other hand, urban particulate and soil standards represent fugitive emission sources such as wind-blown dust, motor vehicular exhaust, and other emission sources in the metropolitan.

Table 1 lists the certified concentrations of the various species in the selected standard sources which serve as input data for the CMB modeling. For chemical species whose concentration was not certified, a 5% relative standard deviation was estimated. Generally, 5% standard deviation is a criterion for duplicate analysis of standard. Based on the certified species of standard particles, the standard deviation of most species is in the range of 1–10%. When the standard deviation is less than 10%, the effect on the model is insignificant and reasonable (data not shown). A total of 23 species, which can be determined in our laboratory, was used to distinguish one source from another.

2.2. Sample preparation

To effectively study the influence of obtained analytical data on the solution of source contributions via the CMB model analysis, 25 simulated samples (in six groups) were prepared. Table 2 lists