Available online at www.sciencedirect.com
ScienceDirect
Atmospheric Environment 41 (2007) 4148–4160
ATMOSPHERIC ENVIRONMENT
www.elsevier.com/locate/atmosenv

Compilation of a database on the composition of anthropogenic VOC emissions for atmospheric modeling in Europe

J. Theloke*, R. Friedrich

Institute of Energy Economics and the Rational Use of Energy (IER), Universität Stuttgart, Hessbruehlstr. 49a, D-70565 Stuttgart, Germany

Received 2 June 2006; received in revised form 20 November 2006; accepted 8 December 2006

Abstract

To analyse and generate air pollution control strategies and policies, e.g. efficient abatement strategies or action plans that lead to a fulfilment of air quality aims, atmospheric dispersion models (CTMs) have to be used. These models include a chemical model, where the numerous volatile organic compounds (VOCs) species are lumped together in classes. On the other hand, emission inventories usually report only total non-methane VOC (NMVOC), but not a subdivision into these classes. Thus, VOC species profiles are needed that resolve total NMVOC emission data. The objective of this publication is to present the results of a compilation of VOC species profiles that dissolve total VOC into single-species profiles for all relevant anthropogenic emission source categories and the European situation. As in atmospheric dispersion models usually modules for generating biogenic emissions are directly included, only anthropogenic emissions are addressed. VOC species profiles for 87 emission source categories have been developed. The underlying data base can be used to generate the data for all chemical mechanisms. The species profiles have been generated using recent measurements and studies on VOC species resolution and thus represent the current state of knowledge in this area. The results can be used to create input data for atmospheric dispersion models in Europe.

The profiles, especially those for solvent use, still show large uncertainties. There is still an enormous need for further measurements to achieve an improved species resolution. In addition, the solvent use directive and the DECOPAINT directive of the European Commission will result in a change of the composition of paints; more water-based and high-solid paints will be used; thus the species resolution will change drastically in the next years. Of course, the species resolution for combustion and production processes also requires further improvement.

Keywords: VOC species profiles; Atmospheric modeling; CTM; Anthropogenic emissions; Traffic; Solvent use; Combustion processes; Production processes

1. Introduction

Volatile organic compounds (VOCs) represent an inhomogeneous substance category; its numerous substances cause various impacts. They are responsible for the increase in ground-level ozone concentrations during sunny summer periods and also for the formation of secondary organic aerosols

*Corresponding author. Tel.: +49 711 685 878 56; fax: +49 711 685 878 73.
E-mail address: Jochen.Theloke@ier.uni-stuttgart.de (J. Theloke).

1352-2310/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.atmosenv.2006.12.026

(Finlayson-Pitts and Pitts, 1999). Furthermore, they contribute to the depletion of stratospheric ozone and to the enforcement of the greenhouse effect. Some components have a carcinogenic, teratogenic or mutagenic character (Wickert et al., 2000). A number of regulations, e.g. various directives of the European Commission, are in force or currently prepared to limit as well the emissions of VOCs as the concentration of secondary pollutants, for example ozone. Especially owing to the highly non-linear relationship between emissions of VOCs and concentrations of secondary pollutants in the atmosphere, the use of atmospheric dispersion models (CTMs) is necessary for identifying air pollution control strategies and policies, e.g. efficient abatement strategies or action plans, that lead to a fulfilment of thresholds. These models include a chemical model, which simulates the chemical transformation of the different VOC species. Owing to limited computer calculation capacity the transformation of the hundreds of different species is not treated separately in the chemistry models; instead individual VOC species are aggregated to groups, their reactivity being a main parameter for the allocation of the single species to these groups. Especially Stockwell et al. (1997) developed a species aggregation method for the regional atmospheric chemistry model (RACM). Other quite often used chemical mechanisms are CBMIV (Gery and Whitten, 1989), Euro-RADM (Stockwell and Kley, 1994), RADM II (Stockwell et al., 1990), EMEP (Simpson, 1992), SAPRC (Carter, 1990, 2000), MELCHIOR (Lattuati, 1997) and the master chemical mechanism (MCM) (Saunders et al., 2003; Jenkin et al., 2003; Pilling et al., 2002).

It is clear that for operating an atmospheric dispersion model, VOC emissions species resolution into classes according to its chemical mechanism are needed. Generally, these data are provided by taking total VOC emissions for the different emission source categories from existing emission inventories and then applying VOC species profiles that express the share, which the different VOC classes have on total VOC. These VOC species profiles are more or less characteristic for the different source categories. Of course, as atmospheric dispersion models are in use, such profiles exist and are applied. However, the profiles used are commonly not published at all or are published only in internal reports; the origin of the data especially is not documented. Thus, there is a need for documented VOC species profiles and it is the objective of this study to provide these.

Previous publications of VOC species profiles include works of Stockwell et al. (1990) and Middleton et al. (1990) for the United States and Orthofer et al. (1991) for Austria. Derwent et al. (1996) published an entire VOC species resolution for the UK. However, the breakdown for emission sources is missing; thus, it cannot be used for scenario calculations with varying shares of different source categories and fewer substances (about 100) were considered than in the present publication. Orthofer et al. (1991) published a VOC species resolution for Austria aggregated to eight reactivity categories, which, however, does not contain some newer results. The same applies for Stockwell et al. (1990) and Middleton et al. (1990). Here, the species resolution refers to the USA. McInnes (1996) does not consider all emission source groups and the species resolution is not very detailed for many emission source groups. Passant (2002) has compiled a very detailed single-species resolution for many source groups for UK.

The objective of this publication is to present the results of a compilation of VOC species profiles for all relevant anthropogenic emission source categories and the European situation. As in atmospheric dispersion models usually modules for generating biogenic emissions are directly included, only anthropogenic emissions are addressed.

2. Approach/method

In the following, species profiles for 87 emission source categories are presented. These emission sources cover all relevant anthropogenic sources of non-methane volatile organic compounds (NMVOC).

To generate these data, information about results of measurements of VOC species were systematically collected and analysed, so that the presented species profiles represent the current state of knowledge. As far as possible, the VOC profiles that have been generated resolved into 306 single species or species classes.

As available results of VOC species resolution measurements are very limited, in many cases information was available only from one country, e.g. Germany, Austria (Orthofer et al., 1991) or the UK (Passant, 2002). Given the common market within the EU, we nevertheless assume that the species resolution presented here can be applied for all EU member countries.

The origin of the data that have been used to prepare the VOC species profiles is described for the