RESEARCH ARTICLE

Screening the emission sources of volatile organic compounds (VOCs) in China by multi-effects evaluation

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HIGHLIGHTS

- · We develop a multi-effect evaluation method to assess integrated impact of VOCs.
- · Enable policy-makers to identify important emission sources, regions, and key species.
- · Solvent usage and industrial process are the most important anthropogenic sources.
- · Styrene, toluene, ethylene, benzene, and m/pxylene are key species to be cut.

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ABSTRACT

Volatile organic compounds (VOCs) play important roles in the atmosphere via three main pathways: photochemical ozone formation, secondary organic aerosol production, and direct toxicity to humans. Few studies have integrated these effects to prioritize control measures for VOCs sources. In this study, we developed a multi-effects evaluation methodology based on updated emission inventories and source profiles, by combining the ozone formation potential (OFP), secondary organic aerosol potential (SOAP), and VOC toxicity data. We derived species-specific emission inventories for 152 sources. The OFPs, SOAPs, and toxicity of each source were estimated, the contribution and sharing of source to each of these adverse effects were calculated. Weightings were given to the three adverse effects by expert scoring, and then the integrated effect was determined. Taking 2012 as the base year, solvent use and industrial process were found to be the most important anthropogenic sources, accounting for 24.2% and 23.1% of the integrated effect, respectively, followed by biomass burning, transportation, and fossil fuel combustion, each had a similar contribution ranging from 16.7% to 18.6%. The top five industrial sources, including plastic products, rubber products, chemical fiber products, the chemical industry, and oil refining, accounted for nearly 70.0% of industrial emissions. Beijing, Chongqing, Shanghai, Jiangsu, and Guangdong were the five provinces contributing the largest integrated effects. For the VOC species from emissions showed the largest contributions were styrene, toluene, ethylene, benzene, and m/p-xylene.

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1 Introduction

Volatile organic compounds (VOCs) comprise thousands of different species, emitting from a wide variety of sources. Hundreds of non-methane hydrocarbons (NMHCs) and oxygenated volatile organic compounds (OVOCs) have significant roles in the formation of ground-level ozone [1]. The photochemistry of various species has been intensively studied since the 1980s, and a method to estimate ozone formation potential (OFP) was developed on the basis of incremental reactivities [2,3].

Some VOCs are precursors of secondary organic aerosols (SOA), and affect air quality, radiation, and cloud microphysics [4]. SOA formed from VOCs account for a large portion of organic particulate matters [5]. In addition to these indirect impacts, species such as 1,3-

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butadiene, benzene, and styrene—are toxic to human beings, causing acute and chronic diseases or exerting carcinogenic or teratogenic effects [6,7]. These effects should be taken into consideration for the top designing of VOC control strategies.

From previous studies, the source types and species were identified for VOCs emission abatement by considering one or two of these effects [8,9]. Using life cycle impact assessment methods for OFP and human toxicity, Laurent and Hauschild determined the most important species affecting human health, and found that there were not correlation between the total impact and VOC emissions [10]. Shin et al. took the ozone and SOA formation potentials of individual VOCs into consideration, and determined the optimum control of VOC constituents and emission sources in Seoul, Korea [11]. Yuan et al. identified the major VOC species in the Pearl River Delta Region by calculating the contributions of each VOC species to the concentration and OFP of total measured VOCs [12]. Lv et al. estimated the SOA formation potential in Beijing summertime, and found that the SOA precursors were present at relatively low atmospheric concentrations and had a low OFP [13]. This indicates that, in addition to VOC emissions and concentrations, OFP, secondary organic aerosol potential (SOAP), and toxicity are all important indicators of VOC regulation. However, few studies have combined these indicators when determining the optimum control strategy.

In this study, we aimed to develop a multi-effects evaluation methodology to enable an integrated effect assessment of VOCs. Using a bulk source-specific inventory in China and available source profiles, emissions of individual species were calculated, and their OFPs, SOAPs and toxicity were subsequently estimated. For each individual effect, the absolute and relative contribution of each source type and provinces were determined in China. Finally, the integrated effect was assessed by giving different weightings to each effect. The multi-effects evaluation proposed in this study can provide support for policy-makers to formulate efficient VOC abatement strategies in terms of key sources, species, and source regions.

2 Methods

2.1 Data sources

2.1.1 Emission inventory and source profile

Each anthropogenic source was classified into one of five categories such as transportation, biomass burning, fossil fuel combustion, industrial processes, and solvent usage, and 15 level-II sources, 61 level-III sources, and 152 level-

IV sources. Using the updated emission factors and sectoral activity data, a VOC emission inventory of China in 2012 was compiled. The detail methodology of the inventory can be found in Bo et al. [14]. The total VOC emission was 2984.7 $\times 10^7$ kg in 2012, to which industrial processes contributed the most (39.3%), followed by transportation (25.6%), solvent usage (14.9%), biomass burning (14.1%), and fossil fuel combustion (6.1%).

VOC source profiles were also collected to assess the chemical reactivity of each source [15]. The source profiles used in this paper were derived from a source profile database for China. A total of 101 source profiles were compiled based upon literatures and real-world tests [16,17] (Appendix A). Each profile was normalized to 75 individual species and 6 groups, including 28 alkanes, 11 alkenes, 1 alkyne, 16 aromatics, 6 halocarbons, 13 OVOCs, and other VOCs. To obtain the species-speciated emission inventories, the 152 sub-sectors were classified into 49 categories, including 9 for transportation, 6 for biomass burning, 9 for fossil fuel combustion, 15 for industrial processes, and 10 for solvent usage, and then gave a reasonable profile for each source (Appendix B). The profiles from measurements in China were preferentially adopted, and profiles from the SPECIATE database of US EPA were used for those sources which we found no national profiles [17]. Almost 80% of the emissions were assigned specific source profiles.

2.1.2 Ozone formation potential (OFP) of VOCs

It is widely recognized that the VOC species differ in their photochemical reactivity [8,18]. Many studies have been conducted for the complex photochemical mechanism of ozone formation, and several methods were developed to quantify the OFP of VOCs. Photochemical ozone creation potential (POCP) and maximum incremental reactivity (MIR) have been widely used to evaluate the contribution of individual VOCs to ozone formation [19,20], and MIR is evaluated to be appropriate for applications in the mixed environment [20]. In this study, the OFP was calculated by multiplying a VOCs emission by its corresponding MIR factor, and the total OFP of a certain sub-sector was then the sum of the OFPs of all species, as shown in Eq. (1):

$$OFP_i = \sum_{j=1}^m E_{ij} \times MIR_j, \tag{1}$$

where OFP_i is the total OFP in the *i*th sub-sector, E_{ij} is the emission of the *i*th sub-sector for the *j*th VOC species, and MIR_j is the maximum incremental reactivity for the *j*th VOC species. The MIR factors for 75 VOC species are updated research result of Carter et al., as shown in Table 1 [21].

Table 1 MIR, SOAP, and toxicity grades of 75 VOC species

species	$MIR/(g O_3 \cdot g^{-1} VOC)$	SOAP ^{a)}	toxicity	species	$MIR/(g O_3 \cdot g^{-1} VOC)$	SOAP ^{a)}	toxicity
ethane	0.281	0.1	0	1-hexene	5.492	0	0
propane	0.489	0	0	ethyne	0.954	0.1	0
i-butane	1.230	0	0	benzene	0.721	92.9	4
n-butane	1.151	0.3	0	toluene	4.005	100	2
cyclopentane	2.392	0	0	m/p-xylene	9.750	84.5	2
i-pentane	1.446	0.2	0	ethylbenzene	3.038	111.6	2
n-pentane	1.313	0.3	0	o-xylene	7.640	95.5	2
methylcyclopentane	2.191	0	0	styrene	1.733	212.3	2
cyclohexane	1.250	0	0	1,2,3-trimethylbenzene	11.971	43.9	1
2,2-dimethylbutane	1.173	0	0	1,2,4-trimethylbenzene	8.872	20.6	1
2,3-dimethylbutane	0.969	0	0	1,3,5-trimethylbenzene	11.763	13.5	1
2-methylpentane	1.502	0	0	i-propylbenzene	2.516	95.5	1
3-methylpentane	1.805	0.2	0	m-ethyltoluene	7.391	100.6	0
n-hexane	1.244	0.1	1	n-propylbenzene	2.025	109.7	1
methylcyclohexane	1.698	0	0	o-ethyltoluene	5.586	94.8	0
2,3-dimethylPentane	1.344	0.4	0	p-ethyltoluene	4.444	69.7	0
2,4-dimethylpentane	1.549	0	0	m-diethylbenzene	7.098	0	0
2-methylhexane	1.190	0	0	p-diethylbenzene	4.431	0	0
3-methylhexane	1.614	0	0	tetrachloromethane	0.000	0	3
n-heptane	1.074	0.1	0	chloroform	0.022	0	3
2,2,4-trimethylpentane	1.261	0	1	dichloromethane	0.041	0	3
2,3,4-trimethylpentane	1.030	0	0	chloromethane	0.038	0	3
2-methylheptane	1.073	0	0	tetrachloroethylene	0.031	0	2
3-methylheptane	1.239	0	0	vinyl chloride	2.827	0	4
n-octane	0.899	0.8	0	formaldehyde	9.456	0.7	3
n-nonane	0.781	1.9	0	aceteldehyde	6.539	0.6	3
n-decane	0.684	7	0	acrolein	7.451	0	2
n-undecane	0.611	16.2	0	propionaldehyde	7.081	0.5	1
ethene	8.995	1.3	1	butyraldehyde	5.974	0	1
propene	11.665	1.6	0	valeraldehyde	5.082	0	0
1,3-butadiene	12.612	1.8	4	isovaleraldehyde	4.972	0	0
1-butene	9.727	1.2	0	benzaldehyde	0.000	216.1	2
cis-2-butene	14.241	3.6	0	hexanaldehyde	4.353	0	0
trans-2-butene	15.163	4	0	acetone	0.356	0.3	0
isoprene	10.607	1.9	1	methyl ethyl ketone	1.481	0.6	1
1-pentene	7.207	0	0	isopropanol	0.614	0.4	0
cis-2-pentene	10.384	3.1	0	ethyl acetate	0.626	0.1	0
trans-2-pentene	10.565	3.1	0				

Note: a) secondary organic aerosol formation expressed on a mass emitted basis as SOAPs relative to toluene = 100

2.1.3 Secondary organic aerosol potential (SOAP) of VOCs

Several smog chamber experiments and model studies have been conducted to estimate SOA formation from the semi-volatile oxidation products of VOCs [22]. The contribution of VOCs to SOA yields has been calculated under different conditions, and it is generally accepted that SOA formation is dominated by a few classes of VOCs, mostly aromatic compounds and monoterpenes, such as benzene, toluene, isoprene and α -/ β -pinene [23,24]. In this study, the current SOAP factors developed by Derwent were used to evaluate the contribution of individual VOCs to SOA yields [25].

The SOAPs listed in Table 1 were developed to define the potential of each VOC to form SOA on a mass basis relative to toluene, as shown in Eq. (2). Although there are specific SOAP factors for only 54 of the 75 species, these species include almost all of the SOA precursors emitted by anthropogenic sources; i.e., aromatics, high-carbon alkanes, and alkenes. Additionally, there are corresponding SOAP factors for 91.2% of the VOCs emitted.

 $SOAP_i =$

Increment in SOA mass concentration with species,j Increment in SOA with toluene

 $\times 100,$ (2)

For the 75 species, the SOAP and emission of an individual VOC was multiplied to estimate its contribution to SOA formation, and the total SOAP of a certain subsector was then defined using the same method as that used for total OFP, as shown in Eq. (3).

$$SOAP_i = \sum_{j=1}^{m} E_{ij} \times SOAP_j.$$
 (3)

2.1.4 Toxicity grading of VOCs

Several dose–response analysis and models have been applied to evaluate the direct toxic effect of VOCs [26,27]. However, no integrated VOC toxicity database was compiled because of the variety of target species and exposure conditions. Thus, we defined toxicity grades for the 75 target species shown in Table 1. The localized toxicity grade of individual VOCs was assigned mainly according to the Registration, Evaluation, Authorization and Restriction of Chemicals, European Union (REACH) VOC categorization decision tree and the VOC control lists of the United States and the European Union [28]. On the basis of information on the carcinogenic, teratogenic, mutagenic properties of different species originating from both the European Commission and the International Agency for Research on Cancer (IARC), the 75 VOC species were categorized into four grades, as follows: grade I, category 1 and 2 carcinogens, mutagens, teratogens, or highly toxic; grade II, category 3 carcinogens, mutagens, teratogens or toxic [29]; and grade IV, harmful or irritant. Toxicity grades 4, 3, 2, and 1 were allocated to grades I, II, III, and IV, respectively.

The toxicity grades and total emissions were multiplied to estimate the relative toxic effect of individual VOCs, and the total relative toxic effect was calculated as described above.

2.2 Multi-effects evaluation method

Many cases have shown that stringent VOCs control measures did help to improve air quality [30], therefore we developed a method to evaluate the environmental effects of VOCs and prioritize VOCs control measures, as shown in Fig. 1. Working with the species-speciated emission inventories of each sub-sector and the MIR, SOAP, and toxicity data, we calculated the absolute contribution of each species in each sub-sector. For the OFP, SOAP, and toxic effect, the total contribution of certain species in all sectors and the total contribution of all species in a certain sub-sector were determined. The relative contribution of each sub-sector and each species was calculated by normalization processing. The integrated effect was determined by taking a weighted average of these three effects, as shown in Eqs. (4) and (5). The multi-effects evaluation system is applicable for different regions and different sectors in China when considering control strategies. We can take both VOCs emissions and



Fig. 1 Multi-effects evaluation method used in this work

(4)

environmental effects into consideration to determine the most important sources and key species.

The weightings of these three adverse effects were assigned by expert scoring. Because O_3 and SOA are crucial for the formation of $PM_{2.5}$ [31,32], and the database was sufficient to quantitatively evaluate the OFP and SOAP of the VOCs, a weighting of 40% was assigned to both of them. There are few methods available to quantitatively evaluate VOC toxicity, and the health effects of VOCs may be related to many toxicological factors [33,34]; therefore, the weighting of VOC toxicity was assigned as 20% to reduce the error. The weighting of OFP, SOAP, and toxicity can be adjusted as information regarding VOCs is obtained. There may be some error when determining the contribution of each source by the multi-effects evaluation method, but it can be used as a guide to screen important VOC emission sources.

Integrated effect of acertain sub-sector = $0.4 \times Relative \ OFP \ contribution$ + $0.4 \times Relative \ SOAP \ contribution$ + $0.2 \times Relative \ toxicity \ contribution,$

Relative OFP contribution
$$= \frac{E_{ij} \times MIR_j}{OFP_i}$$
 (5)

where OFP_i is the total OFP in the *i*th sub-sector, E_{ij} is the emission of the *i*th sub-sector for the *j*th VOC species, and MIR_j is the maximum incremental reactivity for the *j*th VOC species. Relative SOAP contribution and relative toxicity contribution were calculated as described above.

3 Results and discussion

3.1 Contributions of sectors

The most important anthropogenic sources and sub-sectors of each source were determined using the multi-effects evaluation system. Solvent usage and industrial processes were the most important anthropogenic sources, contributing 24.2% and 23.1% of the total environmental effects, respectively. This was followed by biomass burning, transportation, and fossil fuel combustion, all of which had a similar contribution ranging from 16.7% to 18.6%. The contributions listed above were calculated by considering per unit mass VOC emissions, and were significantly different from the VOC contributions of each source as shown in Fig. 2(a). Both the emissions and multieffects of VOCs should be considered when developing abatement measures.

When OFP, SOAP, and the toxic effect were considered separately, there were significant differences among these

sources. In terms of OFP, transportation contributed most, followed by industrial processes, biomass burning, solvent usage, and fossil fuel combustion, with contributions of 29.3%, 24.6%, 21.6%, 17.1%, and 7.3%, respectively. In terms of SOA formation, industrial processes accounted for 42.5% of the SOA mass emissions in China, while solvent usage and transportation accounted for 25.6% and 21.5% respectively, with the contribution of the other two sources being only 10.3%. The toxic effect of industrial processes, biomass burning, and transportation were similar, at 28.0%, 24.7%, and 24.0%, respectively. VOC emissions were taken into consideration when determining each effect. The emission characteristics of the different sources resulted in the differences, not only the actual VOC emissions.

The five largest industrial sources are plastic products, rubber products, chemical fiber products and the chemical industry, and coking, which accounted for nearly 70.0% of the integrated effect (Fig. 2(b)). Emissions from the manufacture of plastic, rubber, and chemical fiber products are very low, but the large number of aromatics emissions from these sub-sectors can lead to significant adverse effects. The integrated effects of different solvent usage sources is shown in Fig. 2(c), with construction accounting for a large part of the integrated effect and VOC emissions, followed by the use of electric machinery and equipment painting, agricultural chemicals, and vehicle painting. These four main sub-sectors accounted for 80.3% of the integrated effect. The VOC emissions and integrated effect of agricultural chemicals are important, but few localized source profiles are available for this source and further study is therefore needed. Light-duty cars and vans were the most important source of transportation, accounting for 54.0% of the integrated effect. Agriculture and architectural off-road mobile sources, and motorcycles contributed 17.5% and 17.0%, respectively (Fig. 2(d)). The integrated effects and VOC emissions of each transportation source were similar, mainly because there were no significant differences in the emission characteristics of the various sources.

3.2 Contributions of VOC species

As shown in Fig. 3(a), the contributions of the various VOCs groups to OFP, SOAP, toxicity, and the integrated effect, were determined. Alkenes and alkynes, and aromatics account for 45.7% and 35.2% of the OFP, respectively, mainly because of the large emission of VOCs and the high MIR. However, alkanes contribute only 6.3% to the total OFP because of their low MIR, while accounts for 21.1% of the total VOC emissions. Almost all of the SOA formation (97.7%) is from aromatic groups, and it is clear that aromatics are important SOA precursors that must be reduced when implementing PM_{2.5} control policies. Aromatics, alkenes and alkynes, OVOCs were all important groups for the toxic effect, accounting for 84.1%



Fig. 2 Contribution of (a) each sector, (b) different industrial sectors, (c) different solvent usage sectors, (d) different transportation sources to the multi-effects and emissions of VOCs

of the total toxicity. It is noteworthy that the emissions of OVOCs and halocarbons were low, but the toxic effects of these two groups were high because of the high toxicity levels of these species. Alkenes and alkynes, and aromatics were the two most important groups, accounting for 84.4% of the integrated effect. Alkanes accounted for 21.1% of all VOC emissions, and their integrated effect was only 2.9%.

The contribution of different VOC groups to the five VOC sources are shown in Fig. 3(b). The alkenes and alkynes, and aromatics are important groups in all five sources, contributing 77.4% to 94.7% of the integrated effects. The integrated effect of solvent usage is mainly from the aromatic group, with a contribution of 91.8%.

The top 10 VOC species contributing to individual effects and integrated effect are listed in Table 2. Ethene, propene, toluene, m/p-xylene, and formaldehyde were the five species that contributed most to ozone formation, with ethene accounting for 21.3% of the OFP. The 10 species that contributed most to SOA formation were all aromatics, including styrene, toluene, benzene, ethyl-benzene, and m/ p-xylene. The 10 aromatics contributed 95.0% of the total

SOAP, with styrene accounting for the largest percentage, at 35.3%. Regarding the toxic effect, the top 10 species accounted for 89.9% of the total toxicity, including ethene, benzene, formaldehyde, vinyl chloride, and toluene. The toxic effect was largely associated with 30 highly toxic species. For the integrated effect, styrene, toluene, ethene, and benzene were the important species whose emissions need to be reduced in China, while the top 10 species accounted for 76.5% of the total integrated effect.

3.3 Contributions of provinces

Using the multi-effects evaluation method, the integrated effect and the three individual effects are determined for different provinces. The top four provinces were Shandong, Guangdong, Jiangsu, and Zhejiang, which accounted for 36.7% together of the total integrated effect. While, Hainan, Ningxia, Qinghai, and Xizang contributed the least, with an overall contribution of 1.3%. This result is consistent with that obtained when the provinces were screened by considering VOC emissions only. Large



Fig. 3 Contribution of the different groups of VOCs to (a) OFP, SOAP, toxicity and the integrated effect, and (b) different VOC sources

emissions of VOCs have a major role in the evaluation of the integrated effect.

To assess VOC emission characteristics and the integrated effect for different regions, we calculated the OFP, SOAP, toxic effect, and the integrated effect per unit mass VOCs emissions of 31 provinces in mainland China (Figs. 4(a)-4(d)), which differ from the result for VOC

emissions shown in Fig. 4(e). As shown in Fig. 4(a), the largest OFP from VOC emissions occurred in Beijing, followed by most regions in the north-east, north-west, and south-west of China. The SOAP from VOCs emissions was concentrated in eastern China, with Chongqing having the highest SOAP. Beijing, Chongqing, Shanghai, Jiangsu, and Guangdong were the top five regions when considering the integrated effect, and the top three regions were all municipalities. The OFP, toxic effect, and integrated effect caused by per unit mass VOCs emissions were most serious in Beijing, possibly because industrial processes, solvent usage and transportation make similar contributions to VOC emissions. Further research regarding the industrial structure in Beijing is required.

3.4 Multi-effects per GDP

The gross domestic product (GDP) of different sectors is also a critical factor used to screen important sources when establishing VOC abatement policies. Based upon the GDP data in 2012, we calculated the integrated effects associated with the GDP for 36 sectors. The sectors were classified according to the classification of national economic industries. For the VOCs emissions per billion CNY of GDP, eight sectors were above 200 t billion CNY^{-1} (Fig. 5(a)), namely chemical fiber products, oil processing and coking, nuclear fuel processing, and rubber products even above 400 t billion CNY⁻¹. For the integrated effect per GDP, the top eight sectors are shown in Fig. 5(b), which are rubber products, chemical fiber products, and plastics products being the most important sectors with a high level of multi-effects/GDP. The important sectors screened by multi-effects and VOCs emissions per GDP unit were similar. These sectors should be given special attention when prioritizing VOC control.

4 Conclusions

In this study, we developed a multi-effects evaluation method based on updated emission inventories of 152

Table 2 TOP 10 VOC species whose emissions need to be reduced in China

species	OFP	species	SOAP	species	toxicity	species	integrated effect
ethene	21.3%	styrene	35.3%	ethene	18.4%	styrene	16.4%
propene	9.3%	toluene	20.2%	benzene	14.1%	toluene	12.8%
toluene	7.4%	benzene	12.8%	formaldehyde	13.1%	ethene	12.3%
m/p-xylene	7.4%	ethylbenzene	8.6%	vinyl chloride	9.4%	benzene	8.3%
formaldehyde	5.7%	m/p-xylene	7.0%	toluene	8.8%	m/p-xylene	6.4%
1,3-butadiene	4.6%	o-xylene	4.7%	aceteldehyde	6.5%	ethylbenzene	4.9%
o-xylene	3.4%	m-ethyltoluene	2.3%	styrene	6.4%	formaldehyde	4.9%
1-butene	3.3%	o-ethyltoluene	1.6%	1,3-butadiene	5.9%	propene	3.8%
aceteldehyde	2.9%	n-propylbenzene	1.4%	dichloromethane	4.3%	o-xylene	3.6%
1,2,4-trimethylbenzene	2.8%	p-ethyltoluene	1.1%	m/p-xylene	3.1%	1,3-butadiene	3.1%



Fig. 4 (a) OFP/emissions, (b) SOAP/emissions, (c) toxicity/emissions, (d) multi-effects/emissions, (e) VOCs emissions of different regions



Fig. 5 (a) VOC emissions and (b) multi-effects associated with the GDP per unit for 15 important sectors

sources and 101 available source profiles, combining OFP, SOAP and toxicity data. The most important emission sources, regions, and VOCs species were proposed.

In terms of the integrated effect, the most important anthropogenic sources were solvent usage and industrial processes, with industrial processes accounting for 42.5% of the SOA mass emissions in China. Plastic products, rubber products, chemical fiber products, and the chemical industry and coking are the most important industrial subsectors that require control in China. The species where control should be prioritized were screened by this method, with alkenes and alkynes, and aromatics having a leading role in all adverse effects and the integrated effect. In addition, styrene, toluene, ethene, and benzene are important species that require control in China. Almost all (97.7%) SOA formation was from aromatic groups.

Special attentions should be given to the sub-sectors with high levels of multi-effects per unit of GDP, such as rubber products, chemical fiber products, and plastics products. The most important regions were screened using the integrated effect caused by per unit mass VOC emissions. Beijing, Chongqing, Shanghai, Jiangsu, and Guangdong were the five regions most in need of control measures, while Chongqing, Zhejiang, Guangdong, Jiangsu, and Tianjin were the most important regions when considering SOA formation only. Further research is needed to determine the industrial structure of these regions, especially Beijing.

Further study is also needed to develop more localized source profiles, so as to derive detailed species-specific emission inventories. In addition to NMHCs, more attention should be given to OVOCs species and halocarbons when compiling profiles. The weightings of the various effects can be adjusted as our knowledge of the characteristics of VOCs species improves, especially with regard to the toxicity of VOCs.

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References

- Shao M, Lu S, Liu Y, Xie X, Chang C, Huang S, Chen Z.Volatile organic compounds measured in summer in Beijing and their role in ground-level ozone formation. Journal of Geophysical Research Atmospheres, 2009, 114(D2):1291–1298
- Carter W P, Pierce J A, Luo D, Malkina I L. Environmental chamber study of maximum incremental reactivities of volatile organic compounds. Atmospheric Environment, 1995, 29(18): 2499–2511
- Atkinson R, Arey J. Atmospheric degradation of volatile organic compounds. Chemical Reviews, 2003, 103(12): 4605–4638
- Kanakidou M, Seinfeld J H, Pandis S N, Barnes I, Dentener F J, Facchini M C, Van Dingenen R, Ervens B, Nenes A, Nielsen C J, Swietlicki E, Putaud J P, Balkanski Y, Fuzzi S, Horth J, Moortgat G K, Winterhalter R, Myhre C E L, Tsigaridis K, Vignati E, Stephanou E G, Wilson J. Organic aerosol and global climate modelling: a review. Atmospheric Chemistry and Physics, 2005, 5(4): 1053– 1123
- Wang S, Wu D, Wang X M, Fung J C H, Yu J Z. Relative contributions of secondary organic aerosol formation from toluene, xylenes, isoprene, and monoterpenes in Hong Kong and Guangzhou in the Pearl River Delta, China: an emission—based box modeling study. Journal of Geophysical Research, D, Atmospheres, 2013, 118 (2): 507–519
- Mølhave L. Volatile organic compounds, indoor air quality and health. Indoor Air,1991, 1(4): 357–376
- Zhou J, You Y, Bai Z, Hu Y, Zhang J, Zhang N. Health risk assessment of personal inhalation exposure to volatile organic compounds in Tianjin, China. Science of the Total Environment, 2011, 409(3): 452–459
- Avery R J. Reactivity-based VOC control for solvent products: more efficient ozone reduction strategies. Environmental Science & Technology, 2006, 40(16): 4845–4850

- Derwent R, JenkinM E, Passant N R, Pilling M J. Reactivity-based strategies for photochemical ozone control in Europe. Environmental Science & Policy, 2007, 10(5): 445–453
- Laurent A, M ZHauschild. Impacts of NMVOC emissions on human health in European countries for 2000–2010: use of sectorspecific substance profiles. Atmospheric Environment, 2014, 85: 247–255
- Shin H J, Kim J C, Lee S J, Kim Y P. Evaluation of the optimum volatile organic compounds control strategy considering the formation of ozone and secondary organic aerosol in Seoul, Korea. Environmental Science and Pollution Research International, 2013, 20(3): 1468–1481
- Yuan B, Chen W, Shao M, Wang M, Lu S, Wang B, Liu Y, Chang C C, Wang B. Measurements of ambient hydrocarbons and carbonyls in the Pearl River Delta (PRD), China. Atmospheric Research, 2012, 116: 93–104
- Lv Z F, Hao J M, Duan J C, Li J H. Estimate of the formation potential of secondary organic aerosol in Beijing summertime. Environmental Sciences, 2009, 30(4): 969–975 (in Chinese)
- Bo Y, Cai H, Xie S. Spatial and temporal variation of historical anthropogenic NMVOCs emission inventories in China. Atmospheric Chemistry and Physics, 2008, 8(23): 7297–7316
- Wei W, Wang S, Hao J, Cheng S. Trends of chemical speciation profiles of anthropogenic volatile organic compounds emissions in China, 2005–2020. Frontiers of Environmental Science & Engineering, 2014, 8(1): 27–41
- Liu Y, Shao M, Fu L, Lu S, Zeng L, Tang D. Source profiles of volatile organic compounds (VOCs) measured in China: Part I. Atmospheric Environment, 2008, 42(25): 6247–6260
- Wei W, Wang S, Chatani S, Klimont Z, Cofala J, Hao J. Emission and speciation of non-methane volatile organic compounds from anthropogenic sources in China. Atmospheric Environment, 2008, 42(20): 4976–4988
- Lu S, Liu Y, Shao M, Huang S. Chemical speciation and anthropogenic sources of ambient volatile organic compounds (VOCs) during summer in Beijing, 2004. Frontiers of Environmental Science & Engineering in China, 2007, 1(2): 147–152
- Derwent R G, Jenkin M E, Passant N R, Pilling M J. Photochemical ozone creation potentials (POCPs) for different emission sources of organic compounds under European conditions estimated with a Master Chemical Mechanism. Atmospheric Environment, 2007, 41 (12): 2570–2579
- Suthawaree J, Tajima Y, Khunchornyakong A, Kato S, Sharp A, Kajii Y. Identification of volatile organic compounds in suburban Bangkok, Thailand and their potential for ozone formation. Atmospheric Research, 2012, 104-105:245–254
- Carter W P. SAPRC Atmospheric Chemical Mechanisms and VOC Reactivity Scales. 2013. Available online athttp://www.engr.ucr.edu/ ~carter/SAPRC/(accessed March 28, 2015)
- Pandis S N, Harley R A, Cass G R, Seinfeld J H. Secondary organic aerosol formation and transport. Atmospheric Environment. Part A, General Topics, 1992, 26(13): 2269–2282
- Matsumoto K, Matsumoto K, Mizuno R, Igawa M. Volatile organic compounds in ambient aerosols. Atmospheric Research, 2010, 97 (1–2): 124–128
- 24. Kroll J H, Seinfeld J H. Chemistry of secondary organic aerosol:

Formation and evolution of low-volatility organics in the atmosphere. Atmospheric Environment, 2008, 42(16): 3593–3624

- Derwent R G, Jenkin M E, Utembe S R, Shallcross D E, Murrells T P, Passant N R. Secondary organic aerosol formation from a large number of reactive man-made organic compounds. Science of the Total Environment, 2010, 408(16): 3374–3381
- Chang C T, Chen B Y. Toxicity assessment of volatile organic compounds and polycyclic aromatic hydrocarbons in motorcycle exhaust. Journal of Hazardous Materials, 2008, 153(3): 1262– 1269
- Ramírez N, Cuadras A, Rovira E, Borrull F, Marcé R M. Chronic risk assessment of exposure to volatile organic compounds in the atmosphere near the largest Mediterranean industrial site. Environment International, 2012, 39(1): 200–209
- European Commission, Joint Research Centre, Institute for Prospective Technological Studies. Reference document on best available techniques in the large volume organic chemical industry. Sevilla, February, 2003
- World Health Organization, International Agency for Research on Cancer. Agents classified by the IARC monographs. 2013. Available online at http://monographs. iarc. fr/ENG/Classification/Accessed

(accessed March 25, 2015)

- Yang L, Wu Y, Davis J M, Hao J. Estimating the effects of meteorology on PM_{2.5} reduction during the 2008 Summer Olympic Games in Beijing, China. Frontiers of Environmental Science & Engineering in China, 2011, 5(3): 331–341
- Mancilla Y, Herckes P, Fraser M P, Mendoza A. Secondary organic aerosol contributions to PM_{2.5} in Monterrey, Mexico: Temporal and seasonal variation. Atmospheric Research, 2015, 153: 348–359
- 32. Song Y, Xie S, Zhang Y, Zeng L, Salmon L G, Zheng M. Source apportionment of PM_{2.5} in Beijing using principal component analysis/absolute principal component scores and UNMIX. Science of the Total Environment, 2006, 372(1): 278–286
- Daisey J, Mahanama K, Hodgson A. Toxic volatile organic compounds in simulated environmental tobacco smoke: emission factors for exposure assessment. Journal of Exposure Analysis and Environmental Epidemiology, 1997, 8(3):313–334
- 34. St. Helen G, Jacob P, Peng M, Dempsey D A, Hammond S K, Benowitz N L. Intake of toxic and carcinogenic volatile organic compounds from secondhand smoke in motor vehicles. Cancer Epidemiology, Biomarkers & Prevention, 2014, 23(12): 2774– 2782