Investigation of plant-level volatile organic compound emissions from chemical industry highlights the importance of differentiated control in China

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Abstract

The chemical industry is a significant source of non-methane volatile organic compounds (NMVOCs), pivotal precursors to ambient ozone (O_3) and secondary organic aerosol (SOA). Despite its importance, precise estimation of these emissions remains challenging, impeding the implementation of NMVOC controls. Here we present the first comprehensive plant-level assessment of NMVOC emissions from the chemical industry in China, encompassing 3,461 plants, 127 products and 50 NMVOC compounds from 2010 to 2019. Our findings revealed that the chemical industry in China emitted a total of 3,105 (interquartile range: 1,179–8,113) Gg of NMVOCs in 2019, with a few specific products accounting for the majority of the emissions. Generally, plants engaged in chemical fibers production or situated in eastern China pose a greater risk to public health due to their higher formation potentials of O_3 and SOA or their proximity to residential areas or both. We demonstrated that targeting these high-risk plants for emission reduction could enhance health benefits by 7%–37% per unit of emission reduction on average compared to the current situation. Consequently, this study provides essential insights for developing effective, plant-specific NMVOC control strategies within China's chemical industry.

Keywords: chemical industry, volatile organic compounds, emission inventory, emission control, plant-level assessment

Synopsis: A plant-level emission inventory of volatile organic compounds was compiled for the chemical industry in China, aiming to prioritize the plants for stringent control measures.

Introduction

Pollution caused by ambient ozone (O_3) and particulate matter (PM) has emerged as a major environmental concern in China,[1–4] resulting in adverse effects on human health, ecosystems and climate.[5,6] Non-methane volatile organic compounds (NMVOCs) are key precursors of O_3 and PM,[7,8] and with successful control of other pollutants like primary PM, SO_2 and NO_x, the role of NMVOCs in deteriorating air quality in China has become increasingly important.[9,10] In 2010, nine ministries in China issued guiding opinions on promoting joint prevention and control of air pollution to improve regional air quality.[11w] These opinions officially introduced the prevention and control of VOCs at the national level. The government and various stakeholders have implemented stringent policies, regulations and measures in industries such as petrochemicals and printing.[12–14] Furthermore, China's 14th Five-Year Plan for the National Economic and Social Development requires a further reduction of nationwide NMVOC emissions by over 10% between 2021 and 2025.[14] Despite these efforts, satellite data has not indicated a decline in NMVOC concentrations,[15] and O_3 and PM pollution persists in China.[16–18] By far, controlling NMVOCs has proven to be a formidable challenge.

A major obstacle to implementing effective NMVOC control is the limited understanding of their emission sources. Unlike many other pollutants that primarily result from combustion processes (e.g., black carbon, nitrogen oxides, sulfur dioxide and carbon monoxide),[19,20] a significant proportion of anthropogenic NMVOCs are attributed to both organized and fugitive emission processes, which may be known or unknown during the production and use of chemicals.[21,22] The chemical industry, which heavily relies on the use of chemicals for its operations, has been identified as a major contributor to NMVOC

emissions.[23,24] Previous studies have estimated the annual NMVOC emission from the chemical industry in China to be in the range of 0.27–2.4 Tg.[24–33] However, these estimates have considerable discrepancies in terms of total magnitude and spatial distribution. These discrepancies are attributed to the following aspects: 1) some studies only considered the manufacturing of a limited number of raw materials (Table S1), while the chemical industry contains a broader range of materials,[34] potentially leading to an underestimation of total emissions; 2) compound profiles are crucial but often missing for certain product production, resulting in an incomplete estimation of individual NMVOC compounds; 3) owing to a lack of plant-specific information, most existing studies use proxies such as population and gross domestic product for spatial allocation, thus introducing biases in the spatial distribution of emissions.[35]

In this study, a detailed inventory of NMVOC emissions from the chemical industry in China was constructed using a comprehensive plant-level dataset. This inventory differs from previously reported inventories in various aspects.[24–33] First, a broader range of raw materials was considered. Second, compound profiles of the emissions were collected for a higher number of products, incorporating as many locally measured profiles from China as possible. Finally, detailed plant-level information, including geographic location, product type, operation status and annual production output, was used to calculate plant-based emissions, which did not exist in previous studies. Covering a broader range of products, local and contemporary data sources, and detailed locations help improve the accuracy of the estimation compared with past studies, furtherly decrease the uncertainty of forecasting of ambient air quality.[36] Based on this emission inventory, O_3 and secondary organic aerosol (SOA) formation potentials were estimated at the compound, sector and

plant levels, which has significant implications for implementing differentiated emission controls in China.

2. Methods

2.1. Overview of the chemical plant dataset

The chemical plant dataset contains comprehensive information on 3,461 chemical plants in China, including their names, operators, participants, operation status, start years, production processes and technologies, exact geographic locations, detailed products and annual production outputs between 2010 and 2019. The dataset was compiled by integrating data from multiple sources (Table S2 and Figure S2), such as GlobalData for names and operators, OpenStreetMap for exact locations and S&P Capital IQ for information on shareholders.[37–39] Further details regarding the integration process can be found in a previous paper.[40]

2.2. Estimation of non-methane volatile organic compound emissions

A bottom-up approach was used to estimate NMVOC emissions for individual chemical plants using the following equations:

$$E_i = A_i \times EF_i \times \left\{ \varepsilon \times \left[\left(1-\eta\right) \times r_j + \left(1-r_j\right) \right] + \left(1-\varepsilon\right) \right\} = A_i \times EF_i \times \left(1-\varepsilon \times r_j \times \eta\right)$$

$$E_{i,k} = E_i \times f_{i,k}$$

where the subscript i denotes the specific plant or province, j denotes the province where the plant is located, k denotes the specific species, E denotes the emissions of total NMVOC or species, A is the annual production output of the plant or the province, EF_i is the emission factor of the specific product produced by plant i, ε is the collection rate of exhaust gas, r is the installation rate of the exhaust gas treating unit in the province, η is the removal

efficiency of the treating unit, and $f_{i,k}$ is the mass fraction of species k in the emission profile of plant or province i. Plants with zero emissions were excluded (mostly plants with zero output or producing inorganic chemical products), resulting in the inclusion of 2,325 plants producing 127 different products in 2019.

The 127 different products were classified into five categories based on their chemical properties, as per the Industrial Classification for National Economic Activities: chemical fibers, fertilizers, raw chemicals, synthetic resins and synthetic rubbers.[34] These products were further divided into four groups based on emission intensity: extremely high-*EF* products with *EF*s higher than 50 g NMVOC per kilogram of products (referred to as ex-high-*EF*), high-*EF* products with *EF*s higher than 10 g kg^{-1} but lower than 50 g kg^{-1} (high-*EF*), medium-EF products with *EF*s higher than 1 g kg^{-1} but lower than 10 g kg^{-1} (medium-*EF*) and low-*EF* products with *EF*s lower than 1 g kg^{-1} (low-*EF*). Detailed information about the products, categories and *EF*s can be found in Tables S3–S5.

The overall uncontrolled *EF*s and compound profiles of NMVOCs were obtained from existing literature and various datasets. For studies exclusively measuring post-treatment *EF*s, we calibrated these *EF*s based on known removal efficiencies (Table S3). These datasets include Technical Guidelines for Compiling Emission Inventory of Atmospheric VOCs Sources for China, the United States Environmental Protection Agency's (US EPA) Compilation of Air Emissions Factors (AP-42) and SPECIATE 5.2.[41–49] The most up-to-date measurements based in China were preferred to enhance the accuracy of the emission estimates. Table S3 provides the list of *EF*s for individual products. For products lacking *EF* measurements, *EF*s with similar chemical structures and production processes were used as alternatives (Table S4, Text S1).

The installation rate of the exhaust gas treating units in China was obtained from the "China Ecology and Environment Yearbook".[50] In a previous study, the removal efficiency of treatment technologies in the chemical industry was measured to be in the range of 60%–90%.[51] As for the collection rate of exhaust gases, the processes of chemical production predominantly take place within completed sealed space, such as reactor vessels. For such sealed spaces, a collection rate of >95% is typically recommended.[52] Additionally, there are fugitive emissions related to the handling and processing of raw materials and other operations. These fugitive emissions have seen significant reductions since the initiation of China's 13th Five-Year Plan for Volatile Organic Compound (VOC) Pollution Prevention and Control in 2017 ("VOC Control Plan").[53] In light of the guidelines and recent stringent controls, we set the collection rate at 85% prior to 2017, progressively increasing it to 95% between 2017 and 2020, aligning with the duration of the VOC Control Plan.[53]

2.3. Calculation of O_3 and secondary organic aerosol formation potentials

Metrics of O_3 formation potential (OFP) and secondary organic aerosol formation potential (SOAFP) were used to evaluate the potential impacts of NMVOC emissions on ambient O_3 and PM formation. OFP measures the contribution of a specific VOC species to O_3 formation and is determined in this study as the maximum incremental reactivity of the VOC species.[54,55] Additionally, SOAFP measures the SOA-forming propensity of a particular VOC species relative to that of an equal mass of toluene multiplied by a factor of 100.[8] These matrices, OFP and SOAFP, are widely used to evaluate the potentials of VOCs in the formation of O_3 and SOA, respectively.[25–27,56,57]

The following formulas show the calculation method for overall OFPs and SOAFPs and when discussing on the OFPs and SOAFPs per unit mass of emissions, they are divided by

the total NMVOC emissions of plants or provinces.

$$OFP_i = E_i \times \sum_k f_{i,k} \times MIR_k$$

$$SOAFP_i = E_i \times \sum_k f_{i,k} \times RTOL_k$$

Where the subscript i denotes the specific plant or province, k denotes the specific species, OFP_i means the O_3 formation potential of the emissions from plant or province i, E_i is the total NMVOC emissions of the plant or province, $f_{i,k}$ is the mass fraction of species k in the emission profile of plant or province i, MIR_k is the maximum incremental reactivity of species k,[54,55] and $RTOL_k$ is the propensities of species k for secondary organic aerosol SOA formation expressed on a mass emitted basis relative to toluene=100.[8]

For an NMVOC mixture emission, the OFP and SOAFP per unit mass of emissions were evaluated by calculating the fraction-weighted averages of the OFPs and SOAFPs of individual NMVOC species, respectively. This enables a direct comparison of these metrics between plants, revealing the differences in the O_3- and SOA-forming capacities of the emissions between plants on a per-unit-mass-of-emission basis. When comparing the O_3 and SOA formation potentials of the overall emissions, these metrics were multiplied by the corresponding emissions of the plants.

2.4. Uncertainty analysis

To illustrate the uncertainty in the final emission estimates for chemical plants, Monte Carlo simulations were used. These simulations were based on the uncertainties in *EF*s (assuming log-normal distribution with a standard deviation determined using the uncertainty of data sources on the $\log_{10}$ scale) (Table S3 and S4), production outputs

(assuming uniform distribution with a coefficient of variation of 20%), collection rate (assuming uniform distribution with a variation of ±3%) and removal efficiencies (assuming normal distribution with a coefficient of variation of 10%).[51,58] A total of 10,000 simulations were conducted to derive the confidence intervals of the final emission estimates. The uncertainty ranges were expressed as interquartile ranges throughout this paper (Figure S1).

2.5. Limitations

Owing to the limitations in data availability, *EF*s and compound profiles of some sources were missing, and were substituted with data from similar sources. Additionally, a simplified scheme for end-of-pipe controls was employed by assuming consistent removal efficiency across different control devices and species. These procedures can be improved to reduce uncertainty when more information becomes available.

3. Results and discussion

3.1. Non-methane volatile organic compounds emissions by product

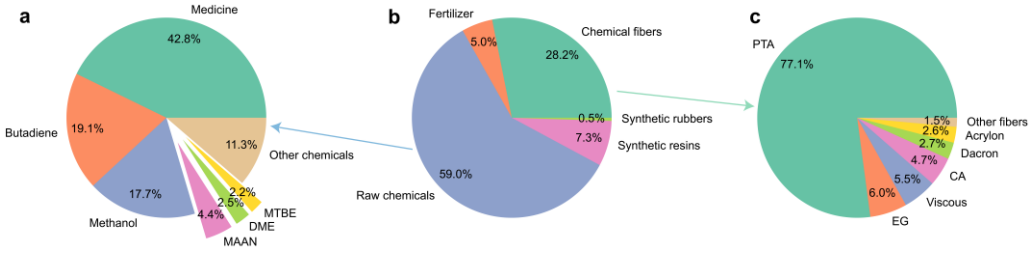

Figure 1. Contributions of individual products to the emissions of non-methane volatile organic compounds (NMVOCs) from the chemical industry in China. a. Contributions of the top six products classified as raw chemicals. **b.** Contributions of the five source categories. **c.** Contributions of the top six products classified as chemical fibers.

Full names of the products are as follows: purified terephthalic acid (PTA), maleic anhydride (MAAN), viscous fiber (Viscous) ethylene glycol (EG), cellulose acetate (CA), dimethyl ether (DME) and methyl tertiary butyl ether (MTBE).

According to our estimates, the total NMVOC emission from the chemical industry in China amounted to 3,105 (interquartile range: 1,179–8,113) Gg in 2019. The five source categories, i.e., raw chemical manufacturing (1,831 Gg, 688–4,824), fertilizer manufacturing (156 Gg, 61–396), synthetic resin manufacturing (227 Gg, 82–578), chemical fibers manufacturing (874 Gg, 335–2,270) and synthetic rubber manufacturing (16 Gg, 6–44), contributed to 59.0%, 5.0%, 7.3%, 28.2% and 0.5% of the total, respectively. Among all products, chemical medicine exhibited the highest emission at 783 Gg, followed by purified terephthalic acid (PTA) at 674 Gg and butadiene at 350 Gg. The emissions of various products were highly dispersed, with a small number of products contributing to the majority of emissions. For instance, the top 14 products with the highest emissions accounted for 88% of the total emissions of 127 products (Table S5).

In terms of *EF*s, ex-high-*EF* products (1,279 Gg, 493–3,250) accounted for 41.2% of the total NMVOC emission, followed by medium-*EF* products (31.8% or 986 Gg, 357–2,726) and high-*EF* products (25.0% or 775 Gg, 301–1,979). Low-*EF* products contributed to only a minor fraction of the total emission (2.1% or 65 Gg, 28–158). Notably, as the *EF* decreases, the production output increases. The total production outputs were 9.7, 61.27, 279.4 and 286.6 Tg for ex-high-*EF*, medium-*EF*, high-*EF* and low-*EF* products, respectively. Although ex-high-*EF* and high-*EF* products accounted for less than one-eighth of the total output, they contributed to more than two-thirds of the total emission. It is worth mentioning that five chemical fibers and six raw chemical products, which are the

predominant contributors to NMVOC emissions (Figure 1b), collectively constitute both ex-high-*EF* and high-*EF* categories. Chemical resins and raw chemical products are pivotal in the medium-*EF* and low-*EF* classifications. The six synthetic rubber products, with *EF* values not exceeding 7.17 g kg^{-1}, are classified as medium-*EF* and low-*EF*, accounting for a mere 0.5% of the total NMVOC emissions.

Our estimate of the total NMVOC emission from the chemical industry in China is 17% to 1,200% higher than that of previous studies (Figure S3a).[24–33] This difference is primarily due to the inclusion of additional emission sources in our assessment. When comparing the same subsets of products, the emission estimates were found to be consistent with those of the previous studies, as shown in Figure S3b, although some differences were evident. For example, our estimate for chemical medicine (1,360 Gg $year^{-1}$) was 248 Gg $year^{-1}$ lower than those in Simayi's study (1,608 Gg $year^{-1}$),[28] whereas the estimate for chemical fibers was 440 Gg $year^{-1}$ higher (955 Gg $year^{-1}$ vs. 515 Gg $year^{-1}$), which is likely due to differences in production outputs. Generally, when comparing overlapping sources, the total-emission estimates are almost identical, with differences from previous studies ranging from −8% to 14%. However, the inclusion of additional sources (i.e., the sources previously unaccounted for) resulted in an extra emission of 625–971 Gg $year^{-1}$, accounting for 22%–27% of the total emission in our estimate. These additional sources include 73 raw chemicals (e.g., methanol with an emission of 325 Gg $year^{-1}$ and maleic anhydride with 81.4 Gg $year^{-1}$), 20 synthetic resins (e.g., polyethylene terephthalate with 17.2 Gg $year^{-1}$), two synthetic rubbers (e.g., polychloroprene with 0.3 Gg $year^{-1}$ and styrene–butadiene–styrene with 0.2 Gg $year^{-1}$) and two chemical fibers (e.g., cellulose acetate with 40.9 Gg $year^{-1}$ and spandex with 1.6 Gg $year^{-1}$). Hence, omitting these sources

significantly underestimates NMVOC emissions from the chemical industry. By covering these sources, the emissions in our estimate were reasonably higher than previous study.

3.2. Compound profile

Figure 2a provides a categorization of the total NMVOC emission into six chemical groups and 18 dominant species. The six groups are alkanes, alkenes and alkynes, oxygenated volatile organic compounds (OVOCs), halohydrocarbons, aromatics, and others. OVOCs represent the dominant group, accounting for 33.5% of the total NMVOC emission. Other groups show comparable contributions, ranging from 8.7% for "others" to 18.3% for alkanes. In terms of species, ethanol is the highest contributor at 16.0%, followed by propane (12.9%) and acetone (11.1%). Several highly toxic species, such as acrylonitrile (0.03%), chloroethylene (0.04%) and 1,4-dioxane (0.3%), show relatively small contributions. It should be noted that these species have higher toxicity levels (measured by Reference Concentration, for example) than most other species.[59] Therefore, their potential contributions to adverse health outcomes are expected to be higher.

Regarding *EF* levels, most compounds emitted from ex-high-*EF* products are OVOCs, whereas alkanes predominantly characterize high-*EF* category emissions. The disparity of six compounds is less in medium category. In the low-*EF* category, aromatics are the primary components, which possess a high potential for SOA formation.[8] More details of the compound profiles by individual product categories are provided in Figure S4.

Figures 2b and 2c show the species contributions to the total OFP and SOAFP associated with the chemical industry. Alkenes and alkynes have the highest contribution on total OFP (56.1%), followed by OVOC (24.3%) and aromatics (13.8%). However, alkanes and others show negligible contributions. Among the species, 1,3-butadiene (34.2%), propene (13.3%)

and ethanol (10.7%) represent high shares. For SOAFP, aromatics make up 97.4% of the contribution, which is far higher than other groups. Styrene (33.7%), benzene (17.2%), ethylbenzene (14.9%) and toluene (14.5%) all show high contributions to SOA formation. Further abatements could focus on these outstanding species to improve efficiencies for O_3 and SOA controls. More details are displayed in Table S6.

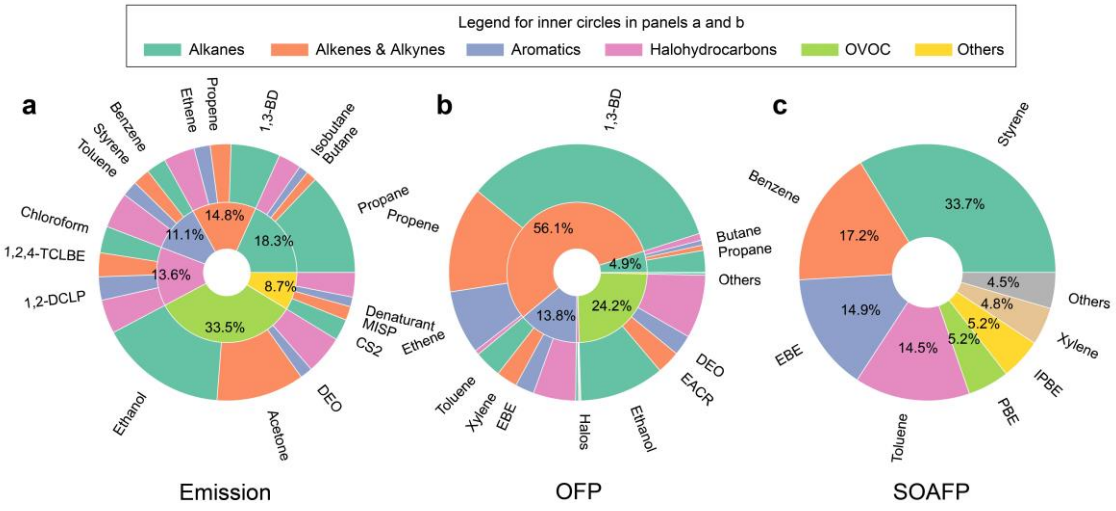

Figure 2. Compound profiles of total NMVOC emission from the chemical industry in China and their relative contributions to O_3 and secondary aerosol formation potentials (OFP and SOAFP). a. Emissions and **b.** OFP categorized into six chemical groups (the inner circle) with 2–3 species for one group (the outer circle). **c**. SOAFP of seven dominant species in aromatics are shown at rank, and species with relatively low contributions are categorized as other species. The abbreviations used in the figure are as follows: 1,3-butadiene (1,3-BD), 1,2-dichloropropane (1,2-DCLP), 1,2,4-trichlorobenzene (1,2,4-TCLBE), ethyl ether (DEO), carbon disulfide (CS2), mineral spirits (MISP), ethylbenzene (EBE), ethyl acrylate (EACR), propylbenzene (PBE) and isopropylbenzene (IPBE).

3.3. Emissions by plant

In terms of emissions by plant, the 2,314 recorded plants accounted for 2,178 Gg year^{-1} (820–5,769) of emissions in 2019, contributing to 70% of the total emission from the chemical industry in China. It should be noted that there is a lack of plant-level information on chemical medicine and chemical fibers. Emissions by plant vary significantly, spanning 10 orders of magnitude. The median and arithmetic mean of the plant-level emissions were 0.17 and 0.94 Gg plant^{-1} in 2019, respectively, with a 95-percentile interval of [0.0013, 3.24] Gg plant^{-1}. Owing to this large inter-plant variation, plants with large emissions disproportionally contribute to the overall emission. For example, the Hengli Petrochemical Dalian PTA Plant, with the highest emission, releases 162 Gg year^{-1} of NMVOCs, which is 173 times the mean level of 0.94 Gg year^{-1} and accounts for 7.5% of the total plant-based NMVOC emission. We found that approximately 31% of the total emission is attributed to only 1% of the plants, and 82% of the plants had emissions less than the mean level. The type of chemical product, production output and emission control are important factors driving the emission variation across plants. This is discussed in the following section.

Among the 119 products (excluding those without plant-level information), the uncontrolled *EF*s range from 0.01 g kg^{-1} for urea to 139.74 g kg^{-1} for butadiene.[41] Plants producing PTA, butadiene and methanol consistently show high emissions (>10 Gg year^{-1}), whereas those producing nitrobenzene, urea and many others show low emissions (<0.1 Gg year^{-1}). Among the top 1% of plants with the largest emissions, 96% produce ex-high-*EF* and high-*EF* products. In contrast, 97% of the plants with lower-than-average emissions

produce medium- and low-*EF* products.

Plants of the same product type exhibit output variations of more than two orders of magnitude, thus affecting the emissions proportionally at the same level of control stringency. Plants producing raw chemicals (by a factor of 1–360) and chemical fibers (5–101) show higher variations in outputs than those producing fertilizer (50–90) and synthetic resins (1–76). The highest variation is found among methanol plants, where outputs vary by a factor of 360 (ranging from 0.01 to 3.6 Tg year^{-1}).

3.4. Spatial distribution

In terms of spatial distribution, 59% of the plants are located in nine eastern coastal provinces (Figure 3), which are also densely populated regions. Compared with inland provinces, coastal provinces generally have higher shares of polluting products (i.e., products associated with ex-high-*EF*s and high-*EF*s) (9.7% and 1.4% of the outputs in coastal and inland provinces, respectively). Consequently, the average uncontrolled *EF* (8.10 g kg^{-1}, determined by products) in coastal regions is 25% higher than that in other regions (6.47 g kg^{-1}). In addition, the whole production output in coastal provinces is 53% more than that in other regions (385 Tg vs. 256 Tg). The combination of higher *EF*s and production outputs leads to intensive NMVOC emissions in coastal provinces. These nine provinces in the coastal region account for 55% of the total emission from all provinces, and a spatial emission density of 1,721 kg km^{-2} in coastal provinces is 9 times higher than that in inland regions (168 kg km^{-2}). Provincial-level emissions and emission densities are displayed in Table S7 and Figure S6.

In inland regions, certain provinces, such as Inner Mongolia (209 Gg year^{-1}), Xinjiang (100 Gg year^{-1}), Henan (114 Gg year^{-1}), Shaanxi (96 Gg year^{-1}) and Hubei (112 Gg year^{-1}),

have high emissions (Figure 3). However, the average uncontrolled *EF*s (6.52 g kg^{-1}) in these provinces are lower than that in coastal provinces (8.10 g kg^{-1}). The high emissions in these provinces can be attributed to their high production output ranging from 9.9 to 37.4 Tg $year^{-1}$, which in the aggregate is more than double the output of all other inland provinces (ranging from 0.006 to 17.0 Tg $year^{-1}$). Subsequent analysis reveals that these provinces are not necessarily highly-industrialized regions (as measured by industrial GDP); rather, they exhibit substantial production of coal and oil, upon which the chemical industry is heavily reliant (Supplementary Text S2 and Figure S7).

It is worth mentioning that Fujian (155 Gg $year^{-1}$), Xinjiang (100 Gg $year^{-1}$) and Inner Mongolia (209 Gg $year^{-1}$) are not located in key control regions introduced by government despite their high emissions (key control regions are shown in Figure S2).[53] Conversely, some provinces within key control regions, such as Hunan (53 Gg $year^{-1}$) and Anhui (43 Gg $year^{-1}$), have relatively low emissions.

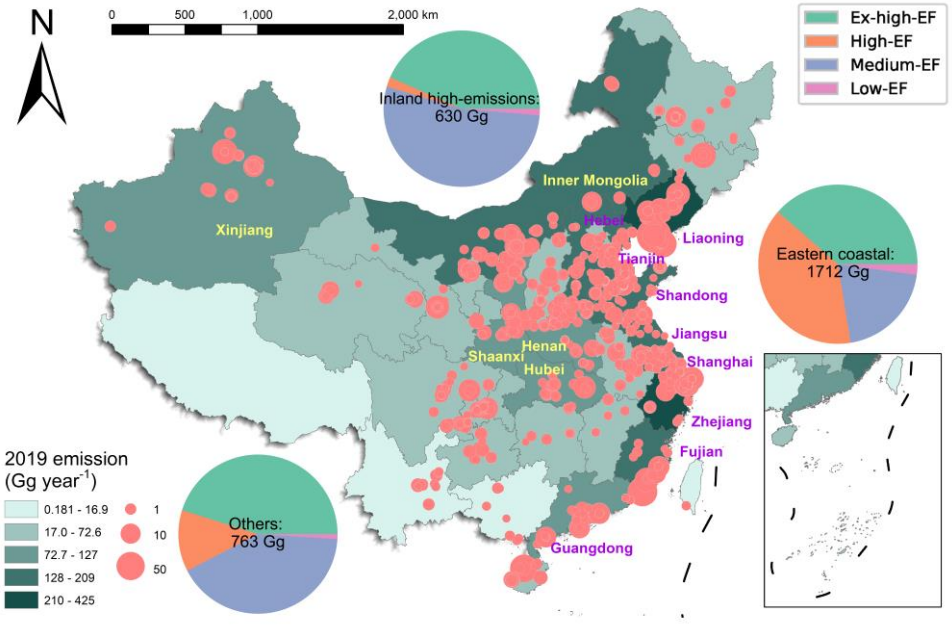

Figure 3. Spatial distributions of NMVOC emissions from the chemical industry in China. The sizes of the circles are proportional to the emissions of the plants, and the background displays provincial-level emissions. The pie charts at the right, top and left demonstrate the total production outputs and the shares of products in eastern coastal provinces (marked by purple font on the map), inland high-emissions provinces (marked by yellow font) and other provinces, respectively. The provincial boundary shapefile was obtained from https://www.resdc.cn/DOI/doi.aspx?DOIid=122.[62]

3.5. Temporal trend

Over time, the annual NMVOC emission from the chemical industry increased from 2,626 Gg in 2010 to 4,142 Gg in 2015, remained stable between 2015 and 2016, and subsequently decreased to 3,105 Gg in 2019 (Figure S8a). This shift in trend observed after 2016 can be primarily attributed to the implementation of more stringent VOC controls and a notable structural shift towards lower-*EF* products. This shift surpassed the growth in production and ultimately led to a decline in emissions. Notably, the total production output nearly doubled between 2010 (322 Tg $year^{-1}$) and 2019 (637 Tg $year^{-1}$), while the policy-guided abatement took effect more significantly since 2017. Consequently, these abatement efforts resulted in a substantial 35% reduction in emissions in 2019, effectively compensating for the emission increase caused by production growth between 2013 and 2019 (Figure S8a). Furthermore, the share of ex-high-*EF* products in the total output decreased from 1.9% to 1.5%, leading to a reduction in the average uncontrolled *EF*s from 8.17 to 7.45 g kg^{-1}, further contributing to a 6% decrease in emissions. In the case of constant output, emissions continued to decrease after 2013 due to the implementation of abatement measures, resulting in a 46% difference compared to the factual emissions in 2019. Figure S8a

provides a comprehensive depiction of the detailed changes in emissions driven by the structure shift, production output and abatement measures.

Emission changes exhibit spatial heterogeneity (Figure S8b). Liaoning, Fujian, Shaanxi, and Hubei have shown significant increases in emissions, whereas Jiangsu, Hebei, Shandong, and Guangdong have experienced substantial reductions. These changes primarily stem from the dynamic interplay between production growth and the efficacy of emission control strategies. For example, in Liaoning, a considerable increase in PTA production output resulted in a noteworthy rise in emissions by 211 Gg $year^{-1}$ from 2010 to 2019. This increase overshadowed the emission reduction of 46 Gg $year^{-1}$ achieved through stringent controls and, coupled with analogous increases in other products, led to a net provincial emission increase of 273 Gg $year^{-1}$. In contrast, in Jiangsu, rigorous emission control, evidenced by an average annual 9.6% increase in the installation of exhaust gas treatment units, led to a significant emission reduction of 371 Gg $year^{-1}$. This decrease exceeded the emission increment due to production growth by 59%, resulting in a net emission reduction of 137 Gg $year^{-1}$, despite generally rising or static trends in the outputs of most products in the province.

3.6. Implications for air quality and public health

Different products exhibit significantly different impacts on air quality owing to variations in their total amount and compound profile. Using two indicators, OFP and SOAFP, the potential impacts of ambient O_3 and SOA formation were assessed from two perspectives: 1) per unit mass of emissions and 2) per overall emissions (Methods). The average OFP per unit mass of emissions is 2.1 g g^{-1}, implying that 1 g of NMVOCs emitted from the chemical industry in China can form 2.1 g of O_3 on average in the atmosphere. Polyvinyl

acetate (PVAc) production has the highest OFP at 15.5 g g^{-1} (Table S5), primarily owing to its significant contribution (99%) of methyl methacrylate (OFP = 15.5 g g^{-1}) in the emission mixture. Following PVAc, the production of styrene–butadiene–styrene (8.3 g g^{-1}) and butyl rubber (6.4 g g^{-1}) have relatively high OFPs per unit mass of emission (Table S5). Conversely, ammonia production has the lowest OFP at 0.1 g g^{-1} (mainly emitting halogenated organic compounds and other species, such as mineral spirits, 1,1,1-trichloroethane and 1,1,2-trifluorotrichloroethane) (Table S5). Notably, the actual amount of O_3 formed by a unit mass of NMVOCs is also sensitive to ambient levels of NO_x.[60] OFP reflects O_3 formation under a NO_x-rich condition,[53] and is therefore a first-order estimate of the NMVOC emission impact on O_3 formation. Thus, OFP merely offers a rough estimation of O_3 formation, rather than a precise evaluation of O_3 produced by NMVOCs.

The average SOAFP of emissions from the chemical industry is 12.7, indicating that the SOA-forming propensity of 1 kg of NMVOCs emitted is equal to that of 0.127 kg of toluene. Note that the SOAFP of toluene is 100.[8] Emissions from the production of expandable polystyrene (EPS) (along with polystyrene) are associated with the highest SOAFP at 202, primarily due to the contribution of styrene (SOAFP = 212) in the emission mixture. It is followed by acrylonitrile–butadiene rubber (126) and ethylbenzene (112) with high SOAFP values (Table S5). The relative differences in SOAFP between products (varying by a factor of 36,372) are more pronounced than those in OFP (varying by a factor of 111). Chemical fibers (such as spandex and viscose fiber) generally tend to have higher SOAFP than the products of other categories ($p < 0.01$ for raw chemicals and synthetic resins, $p < 0.05$ for fertilizers, and $p < 0.1$ for synthetic rubbers by Mann–Whitney U-test).

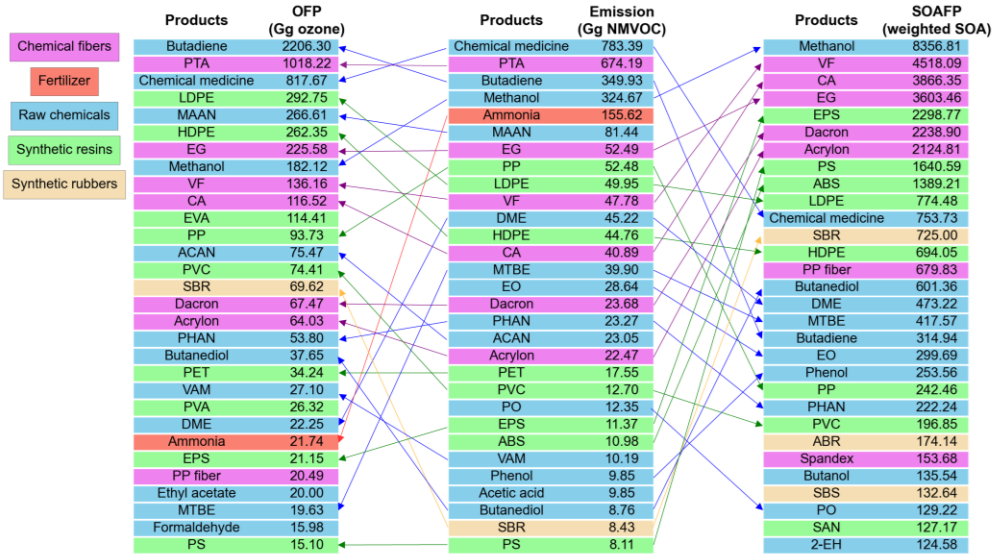

Figure 4. Rankings of the products by emission (in the middle), O_3 formation potential (OFP) (left) and secondary organic aerosol potential (SOAFP) (right) for the chemical industry in China. Only the top 30 products are shown. Full names of the products are as follows: purified terephthalic acid (PTA), maleic anhydride (MAAN), viscous fiber (Viscous) ethylene glycol (EG), polyethylene low density (LDPE), cellulose acetate (CA), polypropylene (PP), polyethylene high density (HDPE), dimethyl ether (DME), methyl tertiary butyl ether (MTBE), ethylene oxide (EO), phthalic anhydride (PHAN), acetic anhydride (ACAN), polyethylene terephthalate (PET), expandable polystyrene (EPS), propylene oxide (PO), polyvinyl chloride (PVC), polystyrene (PS), vinyl acetate monomer (VAM), styrene–butadiene rubber (SBR), ethylene-vinyl acetate (EVA), polyvinyl alcohol (PVA), styrene-acrylonitrile (SAN), acrylonitrile–butadiene rubber (ABR), acrylonitrile–butadiene–styrene (ABS) and 2-ethylhexanol (2-EH).

The rankings of products based on their air quality impacts differ significantly from those based on total emissions due to variations in per-unit-emission OFP and SOAFP values

(Figure 4). For instance, the three products ranking highest in emissions experience a significant decline in SOAFP rankings (11th, 31th and 18th, respectively). Conversely, methanol, viscous fiber and cellulose acetate, which are ranked 4th, 10th and 13th, respectively, in terms of emissions, emerge as the top three contributors to SOAFP due to their higher proportions of high-SOAFP aromatics in the emission mixtures. The SOAFP ranking undergoes a dramatic shift compared to the emission ranking—only one of the top five products with the highest emissions (i.e., methanol) remains among the top five in terms of SOAFP (Figure 4). The ranking based on OFP shows moderate changes compared to the emission ranking. For instance, chemical medicine has the highest emission (783 Gg) but ranks third in terms of OFPs (818 Gg O_3); butadiene has the highest OFP (2,206 Gg O_3) but ranks third in emissions (350 Gg). Ammonia (5th in emissions and 24th in OFPs) and methyl tertiary butyl ether (MTBE) (14th in emissions and 28th in OFPs) exhibit significantly different rankings on emissions and OFPs. This discrepancy is primarily due to the low reactivity of their dominant emission species, namely mineral spirits from ammonia production and 1,2-dichloropropane from MTBE production. Notably, most chemical fibers rank higher in terms of SOAFPs and OFPs than emissions.

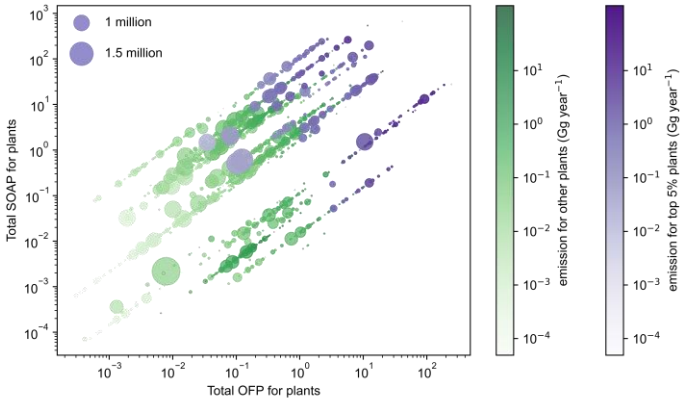

Figure 5. Environmental impact potentials of chemical industrial plants. The points in the figure represent total O_3 and SOA formation potentials of the plants. The colors correspond to total NMVOC emissions from the plants, and the sizes indicate the population residing within a 10 km radius of the plants.[61]

For further analysis, we incorporated population information by multiplying OFPs (or SOAFPs) of individual plants with the population residing within a 10 km radius of the plants.[61] The values were normalized and then defined as the health impact potentials of O_3 and SOA formed by emitted NMVOCs (HP_{O3} and HP_{SOA}), respectively. By doing this, we have assumed that emissions occurring in more densely populated areas are associated with greater adverse public health outcomes. Similarly, we introduced the health impact potential measured by carcinogenic toxicity (HP_{TOX}) which takes into account the 16 of individual VOC species (Supplementary Text S3).[58] The results demonstrate that a small number of plants and a low volume of emissions dominate HP_{O3}, HP_{SOA} and HP_{TOX}. For instance, 1.2%, 2.2% and 0.3% of the plants or 12.4%, 5.8% and 5.7% of the emissions contribute to 50% of the total HP_{O3}, HP_{SOA} and HP_{TOX}, respectively.

We identified the top 5% of plants with the highest HP_{O3}, HP_{SOA} and HP_{TOX}, which are listed in Supplementary Data and represented as blue circles located in the upper right of the scatterplot in Figure 5. These plants are situated in densely populated regions, and are predominantly associated with high OFPs, SOAFPs or high emissions of toxic compounds (Figure S10). Further analysis reveals that 32% of these plants produce high to ex-high-*EF* products (of all of the 2,325 plants, only 7% produce high to ex-high-*EF* products), suggesting that the plants with the most significant public health impacts invariably exhibit the highest emission intensities (Figure S9). Our estimates highlight that targeting

abatement efforts at these plants would be associated with 7% (measured by HP_{SOA}) to 37% (measured by HP_{TOX}) greater health benefits per unit emission reduction, on average, than actual situation. Overall, these top 5% plants account for 73–93% (measured by HP_{O3}, HP_{SOA} and HP_{TOX}) of the overall potential health outcomes induced by the emissions from the chemical industry in China.

Abatement on specific provinces or regions have been appealed in past policies and studies,[24,53] with consideration of emissions, air quality, economics and population. During instances of severe pollution episodes or significant events, local governments often implement enhanced measures to curb emissions, which encompass the temporary suspension of industrial production activities.[63] The implementation of such measures not only presents enforcement challenges but also places a considerable strain on the economy. Our study demonstrates that within the chemical industry, a minority of plants shoulder the primary responsibility for the majority of detrimental consequences on air quality and public health. By directing abatement measures towards these specific plants, it is feasible to enhance practicability and minimize the economic impact, while maintaining the overall efficacy of pollution control endeavors. In conclusion, differentiated controls on individual plants rather than administrative divisions could greatly improve the efficiency of NMVOC controls in the chemical industry, aligning more closely with emission reduction objectives.

Notably, our assessment relies on the utilization of proxies such as OFP and SOAFP, multiplied by population, to approximate potential health impacts. For a more comprehensive understanding, future investigations should employ adjoint analysis within the chemical transport model, allowing for an explicit evaluation of the health consequences associated with thousands of chemical plants in China on an individual basis.

Nonetheless, our findings emphasize the imperative of implementing differentiated controls for chemical plants, given their extensive product range, diverse emission profiles and widespread distribution across China.

Supporting Information contains supplementary tables and figures providing more information on the emission factors adopted in this study, the provincial-level emission estimates and the comparisons with previous studies.

Supplementary Data provides the information on the estimated emissions and health impact potentials of the top 5% plants with the highest HP_{O3}, HP_{SOA} and HP_{TOX}.

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