

Supplementary Materials for

Clean air for some: Unintended spillover effects of regional air pollution policies

Delin Fang, Bin Chen*, Klaus Hubacek*, Ruijing Ni, Lulu Chen, Kuishuang Feng*, Jintai Lin

*Corresponding author. Email: chenb@bnu.edu.cn (B.C.); hubacek@umd.edu (K.H.); kfeng@umd.edu (K.F.)

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1. Schematic methodology

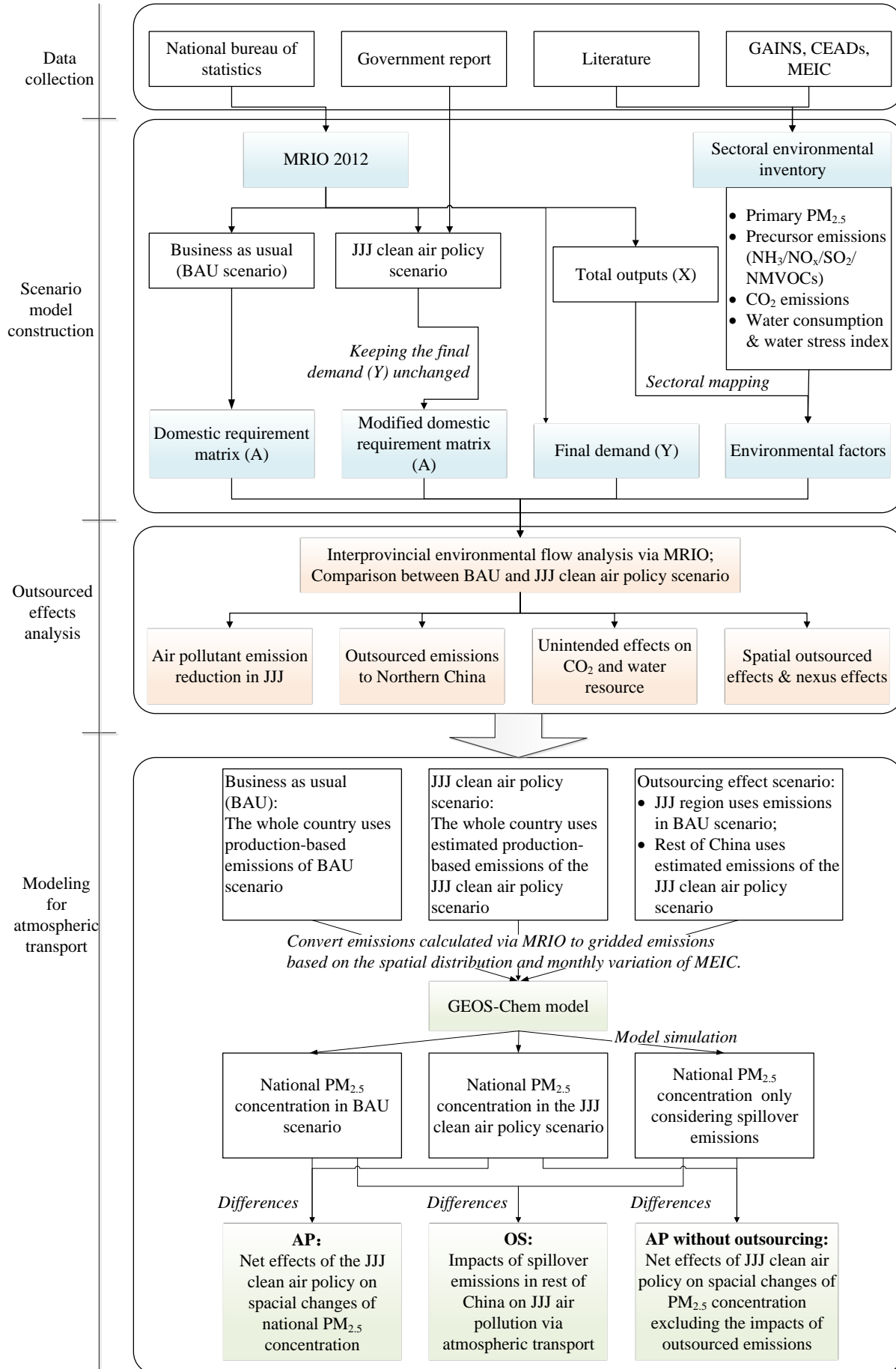


Fig. S1. Schematic methodology for analyzing the spatial spillover and nexus effects of the JJJ clean air policy.

2. JJJ clean air policy

Table S1. JJJ clean air policy measures.

Region	Sector	Measures	2012	2017	Change ratio
Beijing	Coal	By 2017, total coal consumption should be limited to 10 million tons compared to 23 million tons consumed in 2012.	23 million tons	10 million tons	0.435
	Electricity	The share of external electricity input shall be over 70%.	Domestic electricity 71%	Domestic electricity 30%	0.419
			Import electricity 29%	Import electricity 70%	2.38
Nonmetal	Reducing cement production capacity to 4 million tons.	8.8 million tons	4 million tons	0.453	
Tianjin	Coal	Reducing the total consumption of burn coal by 10 million tons. The share of coal in primary energy consumption will decrease to less than 50% by 2017.	52 million tons	42 million tons	0.803
	Electricity	The share of external electricity input will be over 34.71%.	Domestic electricity 82%	Domestic electricity 65%	0.792
			Import electricity 18%	Import electricity 35%	1.98
	Metal	Controlling steel production capacity within 5 million tons.	33 million tons	20 million tons	0.599
	Nonmetal	Controlling cement production capacity within 5 million tons.	7.8 million tons	5 million tons	0.638
Hebei	Coal	Reducing coal consumption by 40 million tons compared with 2012.	300 million tons	260 million tons	0.867
	Metal	Eliminating steel production capacity by 60 million tons.	209 million tons	149 million tons	0.713
		Eliminating iron production capacity by 60 million tons.			
	Nonmetal	Eliminating cement production capacity by 61 million tons. Eliminating 1.8 million tons of glass.	128 million tons	67 million tons	0.523

3. Description of 2012 China multiregional input-output (MRIO) table and spillover index

(a) Description of MRIO analysis

The MRIO table represents the economic structure and the interregional flows of goods and services triggered by the trade network among several interdependent industries and interrelated regions, as well as virtual or embedded flows of associated air pollution (15), carbon emissions(18) and water resources(29, 40), amongst other environmental factors(66)(55). The MRIO approach allows to model policies scenarios and their associated changes in economic structure, interregional flows and final demand, and socio-economic influences and their effects on emissions or resource consumption via explicit representation of environmental coefficients associated with specific economic activities (67, 68). MRIO tables have been widely used for investigations of global or national trade influences on pollution transfers (18, 52, 53, 69). For water resources, MRIO can not only track virtual water flows from final demand to water extraction throughout regional to global supply chains (70), but environmental impacts via the water stress index (WSI) (65). Furthermore, MRIO can facilitate to map patterns of interactions, trade-off and win-win outcomes, between environmental and socio-economic indicators (30, 71).

This study furthers the evaluation of unintended side-effects of regional policy targeting a single environmental issue. We developed scenarios according to the JJJ clean air policy via changing the intermediate process matrix of the MRIO table. The resulting Leontief matrix is utilized to evaluate the spillover effects of emissions and resource transfer via the transboundary trade network. The novelty is in combining virtual or embodied flows of several air pollutants using an MRIO with an atmospheric model, i.e. the nested-grid GEOS-Chem model, that measures actual flows of PM_{2.5} into the study region. The combination of these allows us to assess the actual pollution concentration in JJJ as well as emissions transport from other regions. In addition, it evaluates the unintended effects of JJJ clean air policy with respect to the nexus effects on CO₂ emissions and water resources at regional and the national levels. This study features a holistic picture of the influence of regional policy targeting a single environmental issue, which contains both provincial spillover effects and unintended effects to other environmental issues.

(b) 2012 China MRIO

The 2012 China MRIO table includes 30 provinces, excluding Tibet, Taiwan, Hong Kong, and Macau, is used. The basic data is collected from the national and regional input-output tables of China 2012 (56, 57). The MRIO table is constructed based on 30 regional input-output tables and estimated inter-regional trade flows. The import and export data of each province were used to calculate interregional trade flow matrix of MRIO table via a hybrid technique based on maximum entropy and gravity model(72-74). The MRIO table was calibrated applying the balancing approach RAS method to China's national IO table 2012 via, setting the values from nation IOT as the calibration of the total amount, and the provincial trade flows from the MRIO as the matrix structure. A detailed explanation for the construction of MRIO 2012 can be found in previous studies (58-60).

(c) The MRIO model

In the multi-regional input output model, different regions are connected through inter-regional trade. The technical coefficient submatrix \mathbf{A}^{rs} is defined as

$$\mathbf{A}^{rs} = (a_{ij}^{rs}) = \left(\frac{z_{ij}^{rs}}{x_j^s} \right) \quad (1)$$

in which z_{ij}^{rs} is the intersector monetary flow from sector i in region r to sector j in region s ; x_j^s is the total output of sector j in region s . \mathbf{A}^{rs} is an intermediate consumption matrix where columns reflect the input from sectors in region r required to produce one unit of output from each sector in region s .

The final demand matrix is

$$\mathbf{Y} = (y_i^{rs}) \quad (2)$$

in which y_i^{rs} is the final demand of region s for goods of sector i from region r .

Based on this, the MRIO model can be written as

$$\begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ \vdots \\ x^m \end{pmatrix} = \begin{pmatrix} A^{11} & A^{12} & A^{13} & \cdots & A^{1m} \\ A^{21} & A^{22} & A^{23} & \cdots & A^{2m} \\ A^{31} & A^{32} & A^{33} & \cdots & A^{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A^{m1} & A^{m2} & A^{m3} & \cdots & A^{mm} \end{pmatrix} \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ \vdots \\ x^m \end{pmatrix} + \begin{pmatrix} \sum_s y^{1r} \\ \sum_s y^{2r} \\ \sum_s y^{3r} \\ \vdots \\ \sum_s y^{mr} \end{pmatrix} \quad (3)$$

From this frame work, the extended multi-regional input-output model can be calculated as, which associated with emissions or resources in each region (\mathbf{P})

$$\mathbf{P} = \mathbf{k}(\mathbf{I} - \mathbf{A})^{-1} \mathbf{Y} \quad (4)$$

in which \mathbf{P} represents total emissions or resource consumption to satisfy the production of goods and services along the whole national supply chain triggered by final demands directly and indirectly; \mathbf{k} is a row coefficient vector of emissions or resource consumption for per unit of economic output for all economic sectors; \mathbf{I} is the identity matrix, $(\mathbf{I} - \mathbf{A})^{-1}$ is the Leontief inverse matrix which captures both direct and indirect inputs to satisfy one unit of final demand in monetary value, and \mathbf{Y} is the final demand. \mathbf{P} and \mathbf{k} represent indicators of primary PM_{2.5} emissions, precursor emissions (SO₂, NO_x, NH₃, and NMVOCs), CO₂ emissions and water resources, respectively. Here, we focus on virtual scarce water to analyze spillover effects on water resources, as water extraction creates different impacts depending on the context and underlying initial water stress conditions.

(d) RAS matrix balancing approach

To balance the MRIO table under the JJJ clean air policy scenario, the bioproportional scaling technique, also known as RAS approach, is used to update the input-output table (51).

Step 1: We set the technical coefficient \mathbf{A} matrix of BAU MRIO as the baseline $\mathbf{A}(0)$ matrix. After the JJJ clean air policy scenario adjustment, we get (i) new total gross output vector $\mathbf{X}(1)$; (ii) new total interindustry

(intermediate) sales, by all sectors for sector i , $\sum_{j=1}^n z_{ij}$; and (iii) new total interindustry purchases, by all sector for

sector j this is $\sum_{i=1}^n z_{ij}$.

Step 2: Conventionally, the RAS approach defines $u_i = \sum_{j=1}^n z_{ij}$ and $v_j = \sum_{i=1}^n z_{ij}$, which can be rewritten as $\mathbf{u} = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$

and $\mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix}$. Since these need to be known for the new policy, they will be designated $\mathbf{u}(1)$ and $\mathbf{v}(1)$. Thus, the

RAS procedure addresses that: given an $n \times n$ matrix $\mathbf{A}(0)$ and three n element vectors ($\mathbf{X}(1)$, $\mathbf{u}(1)$, and $\mathbf{v}(1)$), to estimate new $\mathbf{A}(1)$ under the JJJ clean air policy.

Step 3: Starting with row sums, it need to compare the difference between $\mathbf{u}^0 = \mathbf{Z}^0 \mathbf{i} = [\mathbf{A}(0) \hat{\mathbf{X}}(1)] \mathbf{i}$ with $\mathbf{u}(1)$. Set n elements diagonal matrix \mathbf{R} to represent the parameter for adjusting the sum of rows, i.e., $r_i^1 = u_i(1) / u_i^0$ (the subscript in the description of RAS technique stands for the round of adjustment in the procedure), and \mathbf{R} can be written as

$$\hat{\mathbf{R}}^1 = [\hat{\mathbf{u}}(1)](\hat{\mathbf{u}}^0)^{-1} \quad (5)$$

The rows of $\mathbf{A}(0)$ can be rescaled by $\hat{\mathbf{R}}^1$. Thus a first estimate of a \mathbf{A} matrix under the JJJ clean air policy scenario, denoted \mathbf{A}^1 , is given by

$$\mathbf{A}^1 = \hat{\mathbf{R}}^1 \mathbf{A}(0) \quad (6)$$

Here, a better estimate of $\mathbf{Z}(1)$ is obtained, namely $\mathbf{Z}^1 = \mathbf{A}^1 \hat{\mathbf{X}}(1) = \hat{\mathbf{R}}^1 \mathbf{A}(0) \hat{\mathbf{X}}(1)$, with \mathbf{u}^1 that corresponds exactly to $\mathbf{u}(1)$.

Step 4: To check column sums, we need to compare $\mathbf{v}(1)$ and $(\mathbf{Z}^1)' \mathbf{i} = \mathbf{v}^1$. In order to meet the column sum information, n elements diagonal matrix \mathbf{S} is set for the modified parameter to adjust the sum of columns

$$\hat{\mathbf{S}}^1 = [\hat{\mathbf{v}}(1)](\hat{\mathbf{v}}^1)^{-1} \quad (7)$$

Then the second estimate, \mathbf{A}^2 , can be formed as

$$\mathbf{A}^2 = \mathbf{A}^1 \hat{\mathbf{S}}^1 \quad (8)$$

After these adjustments, the column sums are calculated $(\mathbf{Z}^2)' \mathbf{i} = [\mathbf{A}^2 \hat{\mathbf{X}}(1)]' \mathbf{i} = \mathbf{v}(1)$.

Combing Eq. 6 and 8, it would yield

$$\mathbf{A}^2 = \hat{\mathbf{R}}^1 \mathbf{A}(0) \hat{\mathbf{S}}^1 \quad (9)$$

Step 5: By repetition of these adjustment procedures, we would get

$$\begin{aligned} \mathbf{A}^3 &= [\hat{\mathbf{R}}^2 \hat{\mathbf{R}}^1 \mathbf{A}(0) \hat{\mathbf{S}}^1] \\ \mathbf{A}^4 &= [\hat{\mathbf{R}}^2 \hat{\mathbf{R}}^1 \mathbf{A}(0) \hat{\mathbf{S}}^1 \hat{\mathbf{S}}^2] \\ &\vdots \\ \mathbf{A}^{2n} &= [\hat{\mathbf{R}}^n \cdots \hat{\mathbf{R}}^1 \mathbf{A}(0) \hat{\mathbf{S}}^1 \cdots \hat{\mathbf{S}}^n] \end{aligned} \quad (10)$$

The RAS adjustment procedure does converge at a given terminal condition such that all elements in both $[\mathbf{u}(1) - \mathbf{u}^k]$ and $[\mathbf{v}(1) - \mathbf{v}^k]$ are no more than ϵ . Here, we set ϵ as 0.001.

Step 6: Repeating steps 3-5 until terminal conditions are satisfied. Then we get the new technical coefficient matrix \mathbf{A}^{new} and balanced MRIO table for the JJJ clean air policy scenario.

(e) Calculation of spillover index (SPI)

The spillover index (SPI) is calculated by the additional pollution or resource consumption in the rest of China caused by the JJJ clean air policy over the pollution or resource decrease in the JJJ region (without direct pollution and resource reduction from residential activities).

According to Eq. 4, the total emissions or resource consumption for each region to satisfy the production of goods and services along the whole national supply chain under BAU ($\mathbf{P}(\text{BAU})$) and the JJJ clean air policy scenario ($\mathbf{P}(\text{AP})$) can be calculated as

$$\mathbf{P}(\text{BAU}) = \mathbf{k}(\mathbf{I} - \mathbf{A}(\text{BAU}))^{-1} \mathbf{Y} \quad (11)$$

$$\mathbf{P}(\text{AP}) = \mathbf{k}(\mathbf{I} - \mathbf{A}(\text{AP}))^{-1} \mathbf{Y} \quad (12)$$

where $\mathbf{A}(\text{BAU})$ and $\mathbf{A}(\text{AP})$ are the technical coefficient for BAU and the JJJ clean air policy scenario, respectively.

The SPI for sector i can be calculated as

$$SPI^i = \frac{\sum_{r \in \text{Rest of China}} (\mathbf{P}(\text{AP}) - \mathbf{P}(\text{BAU}))_i^r}{\sum_{r \in \text{JJJ}} (\mathbf{P}(\text{BAU}) - \mathbf{P}(\text{AP}))_i^r} \quad (13)$$

where r stands for region r .

4. Policy scenario

The policy scenario is simulated within the framework of MRIO based on the following steps (75, 76):.

Step 1: Keep the final demand of JJJ and rest regions in China unchanged.

Step 2: Scale down the imports of JJJ's sector i of according to the change ratio set by the policy (see last column in Table S1).

Step 3: Calculate the total amount of input reduction of JJJ's sector i and scale up the imports from other regions in China to meet the shortfall.

Step 4: Calculate the increase rest of China's exports to JJJ, and scale up the inputs of sector i in rest of China.

Step 5: Repeat the technique change process of sectors mentioned in Table S1.

Step 6: Using RAS technique to rebalance MRIO matrix.

5. Emission and scarce water consumption factors

(a) Emission factors

The primary PM_{2.5}, SO₂, NO_x, NH₃, and NMVOCs emission inventory is obtained from GAINS model (62). GAINS model provides primary PM_{2.5}, SO₂, NO_x, NH₃, and NMVOCs emission inventories of 59 sectors (77) in 30 provinces of China (78). The data set of PM_{2.5} and its precursors are obtained from ECLIPSE_V5a_CLE_base scenario (2010) in IIASA's GAINS model, which is adopted as a baseline in this study (78). The CO₂ emission factors are calculated based on the CO₂ inventory published by CEADs (64). The classification of the emission inventory and sectoral classification of MRIO2012 table are different. Thus we need to establish a concordance matrix that matches emissions from different classifications and reallocates the emissions to each sector proportional to size (79). Table S2 provides the concordance matrix from GAINS sectors to MRIO sectors.

(b) Scarce water consumption factors

The water consumption intensity factors are provided by Feng *et al.* (29). The sectoral water withdrawal data in each province based on China Economic Census Yearbook (80) and China Water Resources Bulletin (81). Here water consumption refers to the amount of withdrawn blue water that does not return to the ecosystem during a given time period. The ratio of water consumption to water withdrawal is observed in each river basin and for each sector (29), and the water consumption can be calculated by multiplying water withdrawal data with the ratio of water consumption to water withdrawal. The water stress index (WSI) is calculated for the explanation of water stress levels, ranging from 0 (no stress) to 1 (maximum stress), considering water availability, ecosystem type, and climate conditions (65). In this study, we use the WSI calculated by Feng *et al.* (29) for each province in China. For the scarce water consumption calculation, the provincial fresh water consumption is multiplied by provincial WSI in order to reflect the consumption impact on water stress. Then the scarce water intensity coefficient is calculated by the scarce water consumption over total economic output of each sector in each province.

6. GEOS-Chem simulations to analyze impacts of the JJJ clean air policy on ambient PM_{2.5} concentration in China

(a) GEOS-Chem simulation

The impact of the JJJ clean air policy on ambient PM_{2.5} concentration in China is simulated by the nested GEOS-Chem chemical transport model (version 11-01) at a high horizontal resolution of 0.3125° longitude × 0.25° latitude with 47 vertical layers. The model is driven by the assimilated meteorological data of GEOS-FP from National Aeronautics and Space Administration (NASA) Global Modeling Assimilation Office (GMAO; <http://GMAO.gsfc.nasa.gov/>).

Simulations are run with the full Ox-NO_x-CO-VOC-HO_x chemistry and online calculation for various aerosols (secondary inorganic aerosols (SIOA, including sulfate, nitrate, and ammonium), BC, OC, secondary organic aerosols (SOA), dust, and sea salts). SIOA is assumed as being in thermodynamic equilibrium and modeled by

ISOROPIA II (82). Heterogeneous process of sulfate and nitrate follows updates in Zhang *et al.* (34). SOA is estimated based on Liao *et al.* (83) and Marais *et al.* (84). Dry deposition and wet deposition of aerosols follow Zhang *et al.* (85) and Liu *et al.* (86), respectively. Uptake of the hydroperoxyl radical on aerosols follows Lin *et al.* (87). Anthropogenic aromatics are represented by propene as surrogate. Model convection uses a modified Relaxed Arakawa-Schubert scheme and model advection adopts the TPCORE algorithm. The boundary layer mixing is calculated by a non-local scheme (89).

The gridded national anthropogenic emissions of primary PM_{2.5} (excluding BC and OC), NH₃, NO_x, SO₂, CO, BC, and OC in different scenarios (Table S5) are needed to drive GEOS-Chem. Here we develop the gridded emissions with monthly variability based on MEIC v1.2 (89) which contains five major sectors (agriculture, industry, power, residential, and transportation). To aggregate the emissions estimated in our research, we map GAINS emissions sectors and MRIO sectors to MEIC sectors. The mapping matrixes are given in Table S3 and S4. Biogenic emissions are considered in GEOS-Chem by using the Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN v2.1) (90). Soil NO_x emissions follow Hudman *et al.* (91). Biomass burning emissions are taken from Global Fire Emission Database version 4 (GFED v4) (92).

(b) Atmospheric scenarios

In order to illustrate the most extreme results for the PM_{2.5} emission spillover effect, we choose January as an example to present the results, as the pollution status in January is the most serious in most regions. Three nested simulations have been run by covering January in 2012 further with a spin-up period of ten days. The national anthropogenic emissions of primary PM_{2.5}, NH₃, NO_x, SO₂, CO, BC, and OC developed in BAU, AP, and OS scenario (Table S5) were used as emission data inputs for simulations. Model simulations require information of the spatial distributions of emissions from individual sectors.

Simulation SIM_BAU is driven by total emissions over China in the BAU scenario while emissions in simulation SIM_AP and SIM_OS are replaced by estimated emissions in the JJJ clean air policy scenario over the whole China and only the rest of China except JJJ (outsourced emissions), respectively. The difference between SIM_BAU and SIM_AP denotes the impact of the JJJ clean air policy on national PM_{2.5} concentration. A decline of local emissions relieves the air pollution problem in JJJ, but the air pollution transport from outside where emissions increased due to the policy may offset the effect. By comparing SIM_BAU and SIM_OS, we can evaluate the offset impact due to atmospheric transport of increased emissions from outside.

Table S5 Definitions of various atmospheric simulations used in atmospheric transport modeling.

	Definition	Emission data used
SIM_BAU	Business as usual.	The whole country uses emissions in BAU
SIM_AP	JJJ clean air policy scenario.	The whole country uses estimated emissions in the JJJ clean air policy scenario
SIM_OS	Only considering the outsourced emissions in the rest of China.	JJJ region uses emissions in BAU; Rest of China uses estimated emissions of the JJJ clean air policy scenario.
AP	Net effects of the JJJ clean air policy on ambient PM _{2.5} concentration	Compare the differences between the JJJ clean air policy scenario and BAU
OS	Impacts of outsourced emissions to the rest of China on JJJ air pollution via atmospheric transport	Compare the differences between outsourcing scenario and BAU
AP without outsourcing	Impacts of the JJJ clean air policy on changes of ambient PM _{2.5} concentration without the impacts of outsourced emissions.	Compare the differences between AP and OS

7. Emission remapping

In order to facilitate the understanding of the emission estimation processes, this part explains the steps required to remap emission from emission collection, emission estimation for scenarios, gridding of monthly emissions, and

modeling of atmospheric transport. Specifically, we take primary $PM_{2.5}$ emissions in Beijing's electricity sector as an example for detailed explanation.

(a) Emission data collection

The emission data inventory of primary $PM_{2.5}$ and its precursors are collected from IIASA's GAINS model, including 59 sectors in 30 provinces of China (see supplementary materials, part 5).

E.g.: Primary $PM_{2.5}$ emissions for the electricity sector of Beijing are collected from GAINS sector Public electricity and heat production (first column of Table S2).

(b) Scenario model construction

According to the JJJ clean air policy requirement (supplementary materials, part 2), we establish the policy scenario based on the MRIO approach and RAS technique (supplementary materials, parts 3 and 4), and calculate the new technical coefficient matrix (A matrix) of the JJJ clean air policy scenario. This allows us to calculate the adjusted MRIO table that represents the JJJ clean air policy scenario.

E.g.: The domestic production of the electricity sector in Beijing are reduced, while the electricity imports for Beijing from other regions are scaled up. After the adjustment of all sectors according to the policy requirement, the MRIO matrix is balanced via RAS approach, and the new MRIO table based on the JJJ clean air policy scenario is calculated.

(c) Emissions of BAU and JJJ clean air policy scenarios

Emissions of BAU scenario are based on the emission inventory from GAINS, which provides detailed sectoral emissions of each province in China. The classification of the emission inventory and sectoral classification of the MRIO table are different. The concordance matrix (Table S2) is established to match the emissions from the GAINS sectors to MRIO sectors (supplementary materials, part 5). Based on the detailed emission information provided by GAINS and total outputs of each sector and province from the MRIO, we can calculate the emission intensity of each sector in each province of China. Considering the JJJ clean air policy, emissions of different scenarios can be estimated as the adjusted MRIO matrix multiplied by the vector of emission intensities of each sector (see Eq. 4).

E.g.: Primary $PM_{2.5}$ of Beijing's electricity sector in BAU scenario, collected from sector (1) Public electricity and heat production of GAINS, are mapped to sector (25) Electricity and steam production and supply in MRIO. The primary $PM_{2.5}$ intensity (amount of $PM_{2.5}$ emissions per unit of economic output) of Beijing's electricity sector is calculated by dividing sectoral emissions by total output of the electricity sector given in the MRIO. Primary $PM_{2.5}$ of Beijing's electricity sector in the JJJ clean air policy scenario is evaluated by multiplying the emission intensity of the electricity sector with the adjusted MRIO table.

(d) Gridded monthly emissions

To drive the atmospheric chemical transport model GEOS-Chem, province-based emissions need to be converted into gridded emissions. Since MEIC provides monthly gridded emissions for 2012, we converted emissions calculated via MRIO to gridded emissions based on the spatial distribution and monthly variation of MEIC (supplementary materials, part 6).

Three steps are taken to derive gridded emissions. Firstly, we mapped the 42 sectors of the MRIO to the 5 main sectors used in MEIC (using the concordance matrix, Table S4). Secondly, for each sector of each province, we calculated the ratio of yearly emissions estimated in this study to the equivalent sector from MEIC. Finally, we applied the ratio as a scaling factor to monthly gridded emissions from MEIC with the resolution of 0.25° long. \times 0.25° lat. Here, we assumed that the spatial distribution of emissions of each sector in each province remains unchanged before and after the JJJ clean air policy.

E.g.: The primary $PM_{2.5}$ emissions of Beijing's electricity sector in both BAU and the JJJ clean air policy scenarios are mapped to the electricity sector used in MEIC. For Beijing, we calculated the ratio of yearly electricity emissions estimated in this study to that from MEIC. This ratio is applied as a scaling factor to monthly gridded emissions from MEIC with the resolution of 0.25° long. \times 0.25° lat, so as to grid the primary $PM_{2.5}$ emissions from Beijing's electricity to cells in every month.

(e) Modeling atmospheric transport

We use GEOS-Chem simulations to analyze impacts of JJJ clean air policy on ambient $PM_{2.5}$ concentration in China in January. We define three types of atmospheric simulations, including SIM_BAU, SIM_AP, and SIM_OS. The differences between these simulation results reflect impacts of the JJJ clean air policy on national ambient $PM_{2.5}$ concentration, as well as the influence of outsourced emissions on JJJ region (supplementary materials, part 6).

E.g.: The gridded emissions in both BAU and clean air policy scenarios are utilized to drive the atmospheric chemical transport model GEOS-Chem.

8. Spillover effects of the JJJ clean air policy

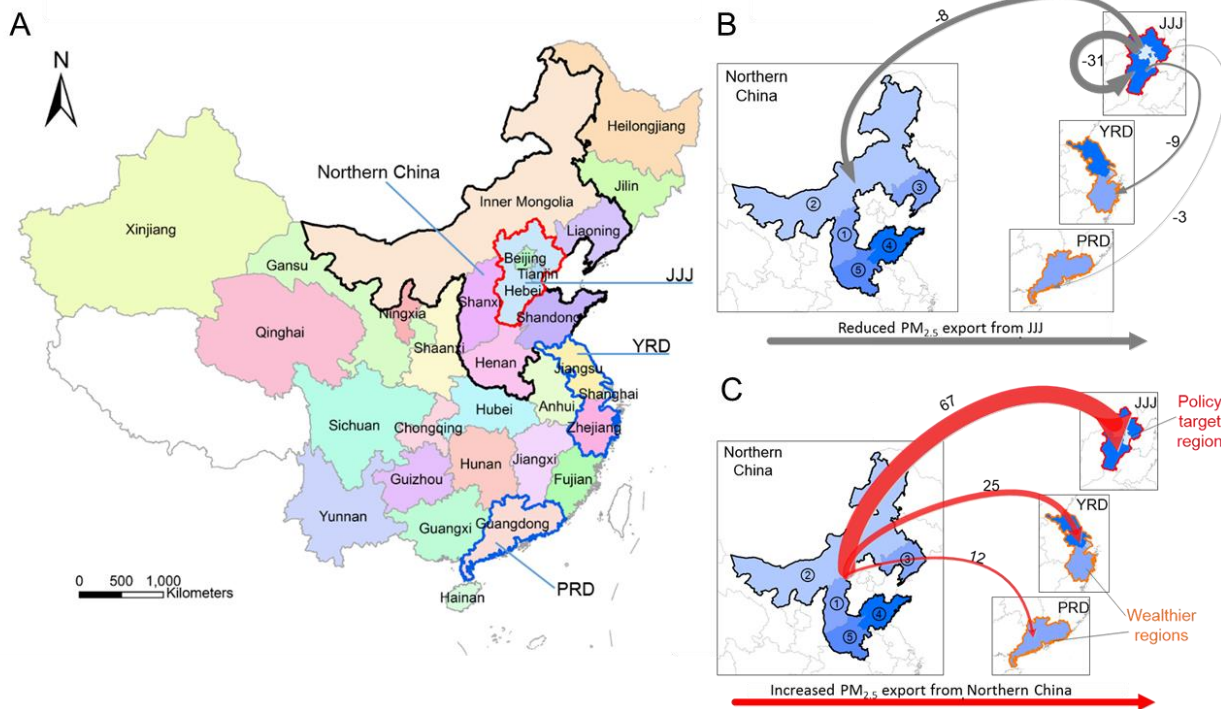


Fig. S2. PM_{2.5} spillover effects of the JJJ clean air policy at the regional level. (A) Names of China's provinces and regions; (B) Reduced embodied PM_{2.5} exporting from JJJ; (C) Increased embodied PM_{2.5} exporting from Northern China. ① Shanxi, ② Inner Mongolia, ③ Liaoning, ④ Shandong, ⑤ Henan.

9. Atmospheric simulation results

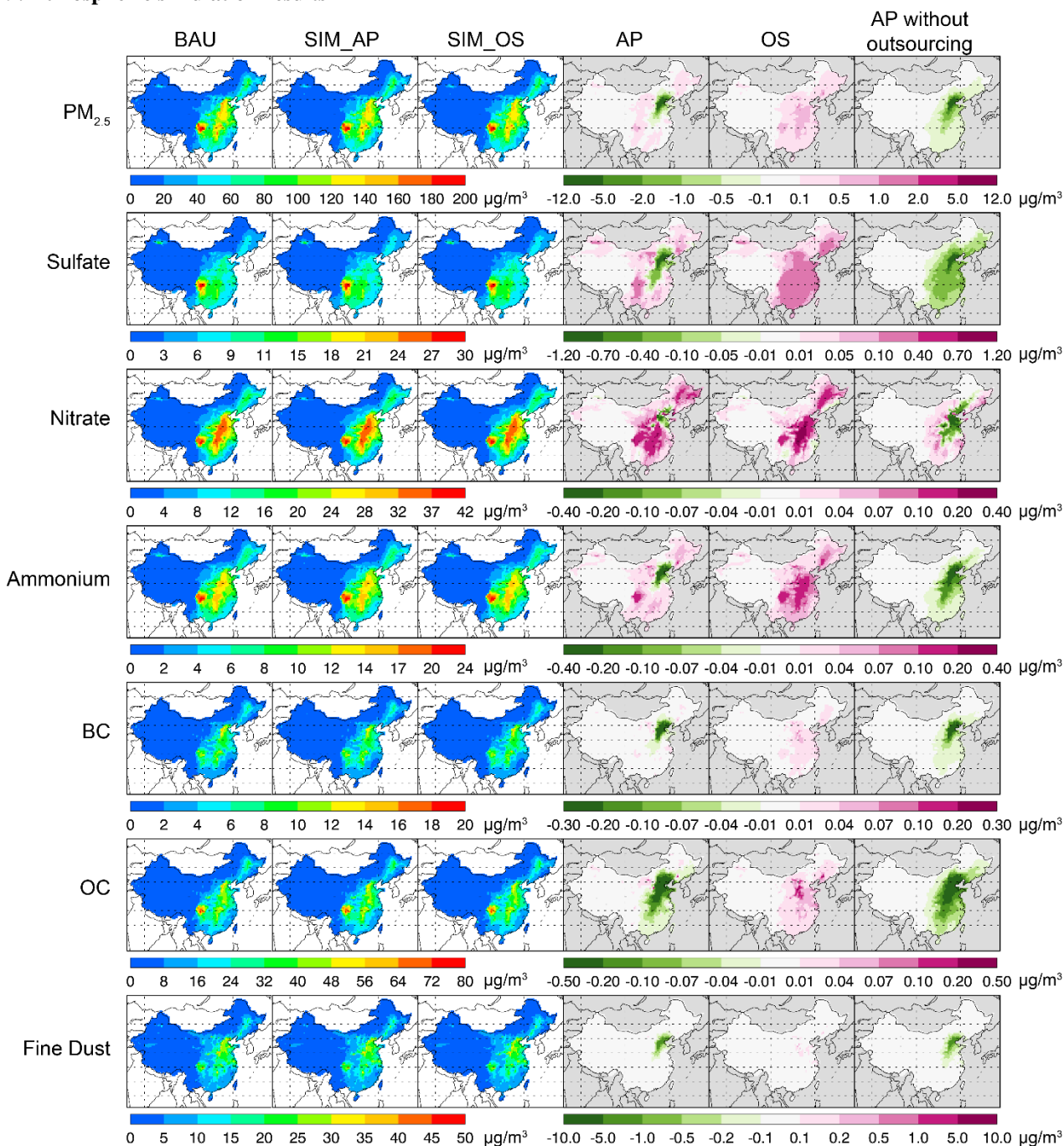


Fig. S3. Simulated surface air pollution in China.

10. Uncertainties and limitations

There are uncertainties and limitations of our research concerning the estimation of emission inventory, underlying assumptions of the air pollution control scenario and spillover index, and modelling of atmospheric transport.

(a) Emission inventory estimation

The emission inventory of this study is collected from the GAINS model (62). GAINS attempts to provide a comprehensive account of emissions of human activities. GAINS faces uncertainties due to methodological issues, insufficient data, and incomplete information of economic activities, energy utilization and emission reduction measures (93). Fig. S4 provides the comparison of production-based emission (PM_{2.5}, SO₂, NH₃, NO_x, and NMVOCs) estimates between this study (2010) and Multi-resolution emission inventory for China (MEIC v.1.2, 2010) (63) by

sector and by region in China. The uncertainties are larger for NH_3 and NO_x emissions compared with $\text{PM}_{2.5}$, SO_2 , and NMVOCs emissions.

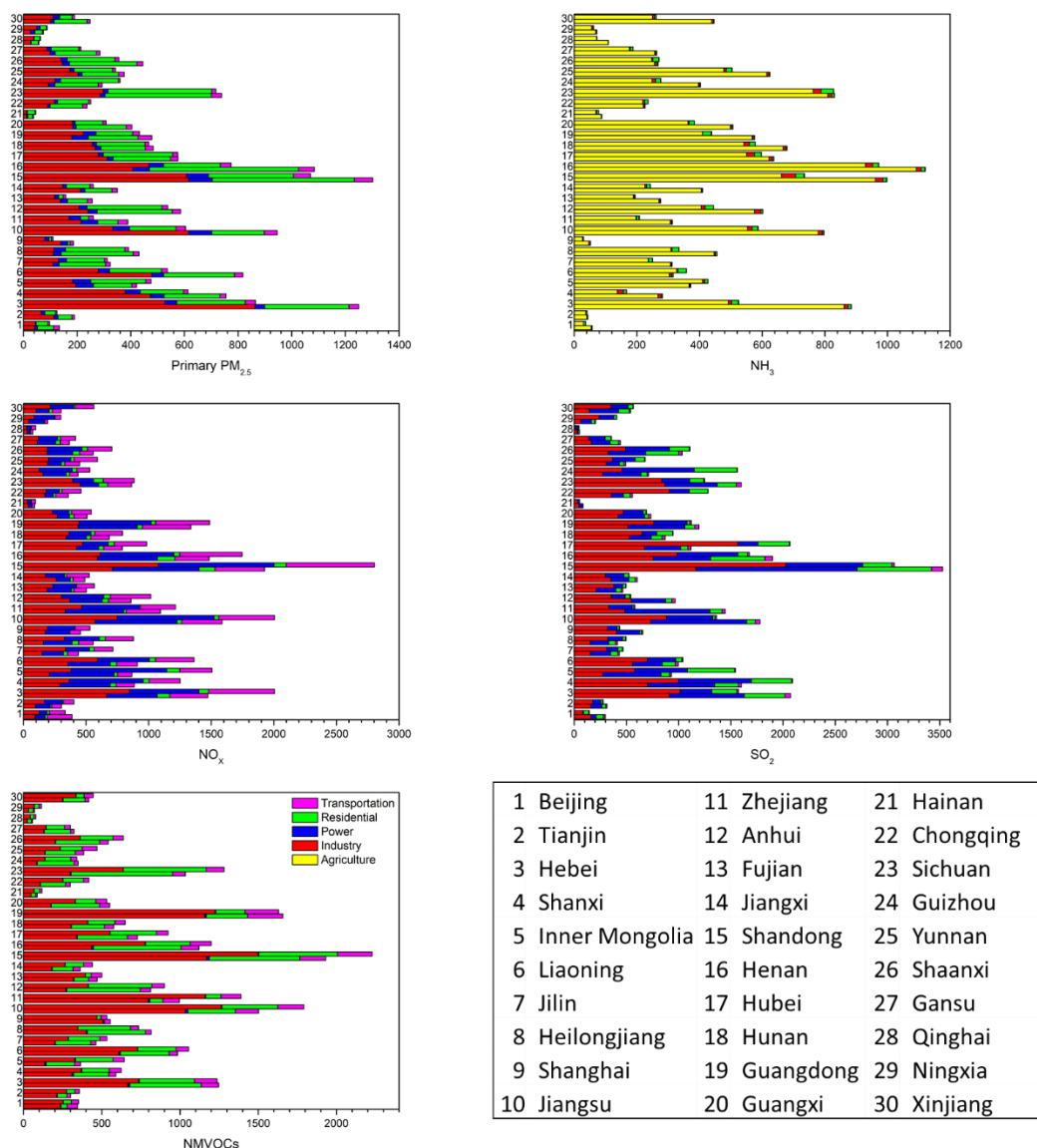


Fig. S4. Comparison of production-based emission estimates of this work (2010) and MEIC v.1.2 (2010) by sector and by region.

(b) Assumptions for JJJ air pollution control scenario and spillover index

The JJJ clean air policy scenario is established according to government documents on JJJ clean air policy, such as the “Air pollution prevention and control action plan” (14) and “The action plan for the implementation of air pollution control rules in Jing-Jin-Ji” (17). The change ratio of each targeted sector is calculated based on current production and the calculation of predicted reduction in production in JJJ region. The production shifts from JJJ to other regions are estimated based on the JJJ clean air policy combined with the MRIO 2012 economic production and trade structure. Such estimated production capacity transfer presents only an approximation and thus might introduce uncertainties of the JJJ air pollution control scenarios. However, this might provide the best estimate given the current available data.

There are a few sources of uncertainties with regards to environmental input-output analysis. The allocation of emissions to economic sectors is based on fixed emissions coefficients per unit of output, which is a reasonable assumption in the short-run.

Allocating production-based emissions to the regions where goods and services are finally consumed using technical coefficient **A** matrix in MRIO generates additional uncertainties, related to sectoral aggregation and inconsistent statistics. However, it is very difficult to assess the uncertainty with regards to the MRIO analysis. In this study, we use the common approach to compare our modeling with result with existing studies. Our comparisons between different MRIO modeling results shows that that the MRIO approach used in our study provides consistent results with previous studies (supplementary materials, part 11).

(c) Spillover index (SPI)

The calculation of SPI is subject to uncertainty of emissions estimated in the JJJ clean air policy scenario, i.e. spillover emissions to the rest of China. In order to capture the range of SPI, the assumed maximum and minimum scenarios provide the extreme values of what could potentially happen in terms of outsourced production and new trade connections. The extreme values are calculated in that we choose the region around JJJ with the highest emission intensity and lowest emission intensity to which JJJ could potentially outsource. Specifically, only the emission intensities of regions around JJJ including Shanxi, Inner Mongolia, Shandong, Liaoning, and Henan, are taken into consideration. Under the JJJ clean air policy, the emissions are mainly outsourcing to these regions, and they have strong connections with JJJ both economically (trade activity) and geographically (distance).

Maximum SPI scenario: We assume that all emissions and resource consumption are outsourced to the region with the highest intensity. Specifically, based on Eq. 13, the largest emission/resource consumption intensity for sector i in regions of Shanxi, Inner Mongolia, Shandong, Liaoning, and Henan, is selected as

$$k(\max)_i = \max(k_i^{\text{Shanxi}}, k_i^{\text{Inner Mongolia}}, k_i^{\text{Shandong}}, k_i^{\text{Liaoning}}, k_i^{\text{Henan}}) \quad (14)$$

Then we set the derived largest intensity as the intensity of sector i for each region in the rest of China

$$k_i^{r, r \in \text{Rest of China}} = k(\max)_i \quad (15)$$

Using the new matrix **k**, we can calculate the upper bound value of SPI for each sector.

Minimum SPI scenario: as opposed to the maximum SPI scenario, we assume that all emissions/resource consumption are outsourced to the region with the lowest intensity.

Accordingly, the calculated upper and lower bars in Fig. 6 illustrate the uncertainty level correlated with SPI.

(d) Modelling of atmospheric transport

The calculation processes of the PM_{2.5} concentration by the atmospheric chemical transport model GEOS-Chem are influenced by uncertainties related to sectoral emission inventories and the model characterization of atmospheric chemical and physical processes, such as secondary organic aerosols, vertical transport, and deposition and scavenging (9). The computational intensity of the GEOS-Chem model makes it impracticable to evaluate correlated uncertainties by a sensitivity analysis.

Instead, we utilized the normalized root-mean-square deviation (NRMSD) between the observed data reported hourly by the Ministry of Environmental Protection in China (MEPC, <http://106.37.208.233:20035/>) and the simulated PM_{2.5} concentrations to illustrate the overall model errors for each region China. At least 20 valid hourly records with in a day are required to calculate daily means. Based on the valid daily mean records, at least 80% valid daily mean records are required to calculate monthly mean PM_{2.5}. For model evaluation, we conduct one more simulation with anthropogenic emissions derived from the data inventory used in this study. Model data sampled are congruent with valid measurements data both at the times (based on hourly data) and locations.

Fig. S5a compares the modeled monthly mean PM_{2.5} to the observations over the whole of China. Our model underestimates PM_{2.5} concentration by 4% due to the limited capacity of simulating secondary organic aerosols. The model reproduces the spatial distribution of PM_{2.5} well with a high correlation coefficient (R) of 0.72. For

comparisons over JJJ (Fig. S5b), the model results show a small bias with measurements (with normalized mean bias of 4% and with a high R of 0.83). These agreements between model and observations give us confidence of source-receptor simulations.

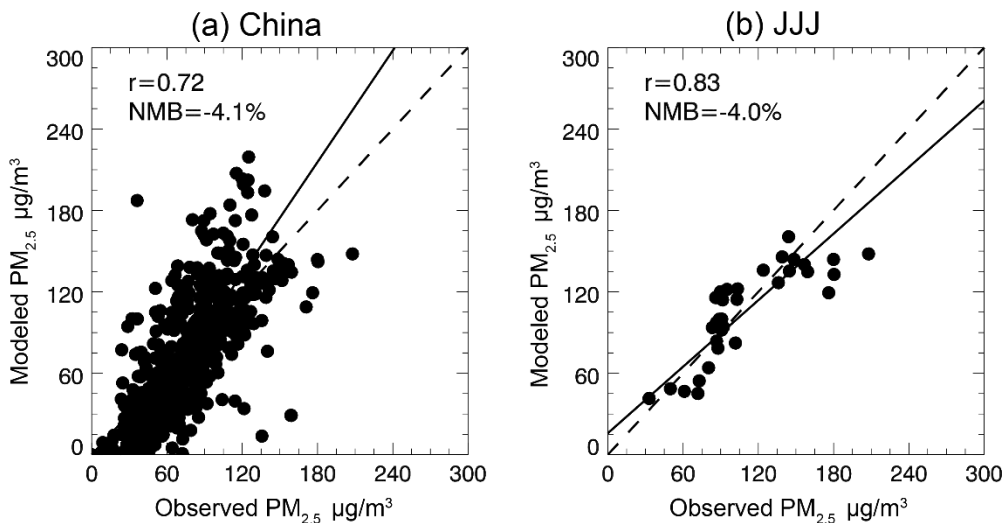


Fig. S5. Comparisons between the simulated and observed monthly mean PM_{2.5} concentration over (a) China and (b) JJJ region.

11. Comparison with other studies

The provincial transboundary transport of primary PM_{2.5}, NO_x, SO₂, and NMVOCs was investigated by Zhao et al. (16). A detailed comparison is given below:

(1) The research of Zhao et al. (16) utilized the MRIO for 2007 and emissions inventory from MEIC2010 (94) to investigate China's virtual air pollution (primary PM_{2.5}, NO_x, SO₂, NMVOCs) transport embodied in provincial and trade. Fig.S6 is the comparison between the research of Zhao et al. (16) and this study.

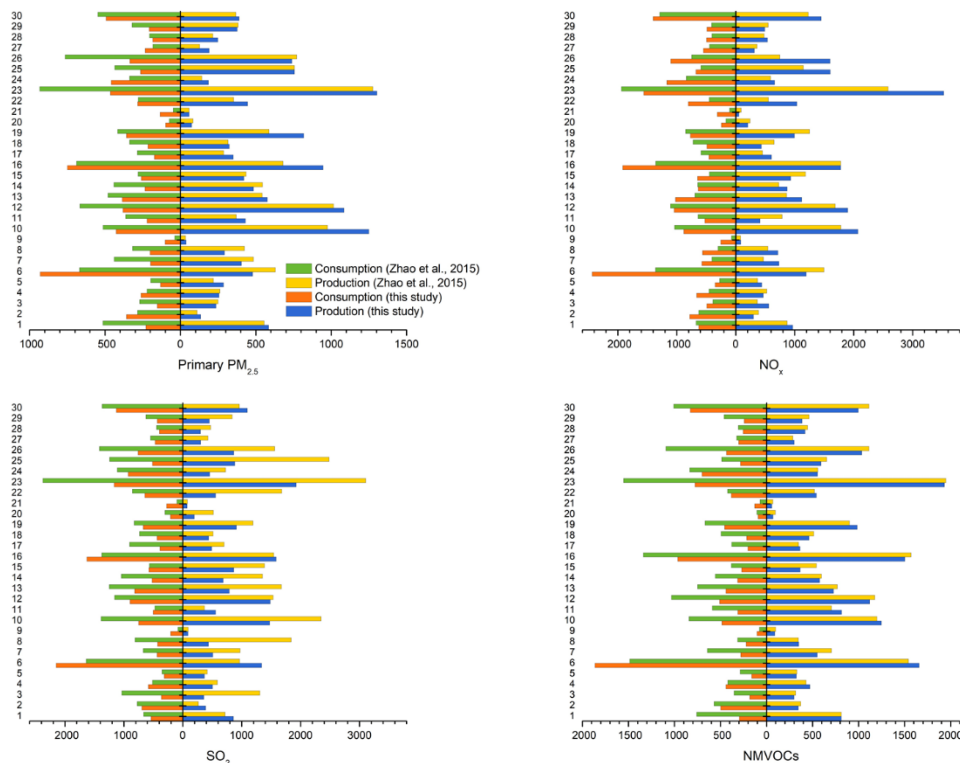
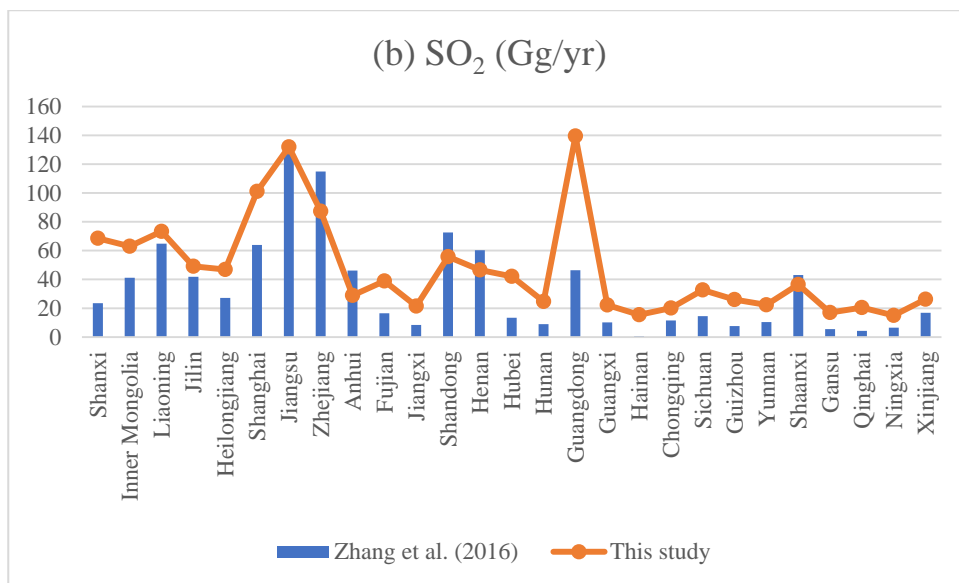
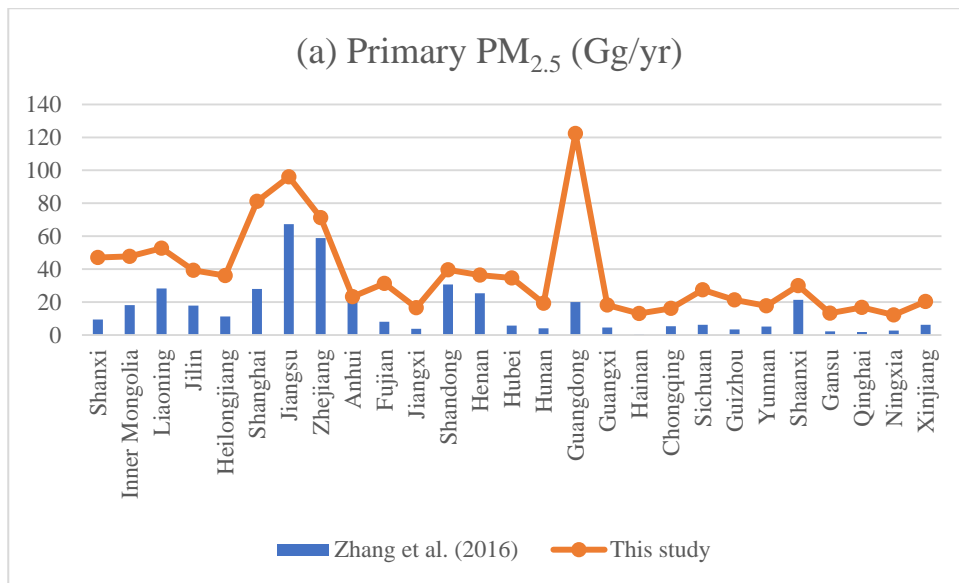


Fig. S6. Comparison of regional pollutant emissions from production- and consumption-based perspective (kt year⁻¹). In each panel, bottom bars show the emission estimated in this work and top bars represents the emissions

calculated in the research of Zhao et al. (16). (The numbers in the column represents provinces and cities in China: 1-Anhui, 2-Beijing, 3-Chongqing, 4-Fujian, 5-Gansu, 6-Guangdong, 7-Guangxi, 8-Guizhou, 9-Hainan, 10-Hebei, 11-Heilongjiang, 12-Henan, 13-Hubei, 14-Hunan, 15-Inner Mongolia, 16-Jiangsu, 17-Jiangxi, 18-Jilin, 19-Liaoning, 20-Ningxia, 21-Qinghai, 22-Shaanxi, 23-Shandong, 24-Shanghai, 25-Shanxi, 26-Sichuan, 27-Tianjin, 28-Xinjiang, 29-Yunnan, 30-Zhejiang)

(2) The research of Zhao et al. (15) utilized the environmental input-output analysis for 2010 to evaluate the air pollutants (primary $PM_{2.5}$, SO_2 , NO_x , and NMVOC,) associated with interprovincial exports from JJJ. Here we compare the SO_2 emission flows exported from JJJ driven by transboundary trade (Fig. S7).



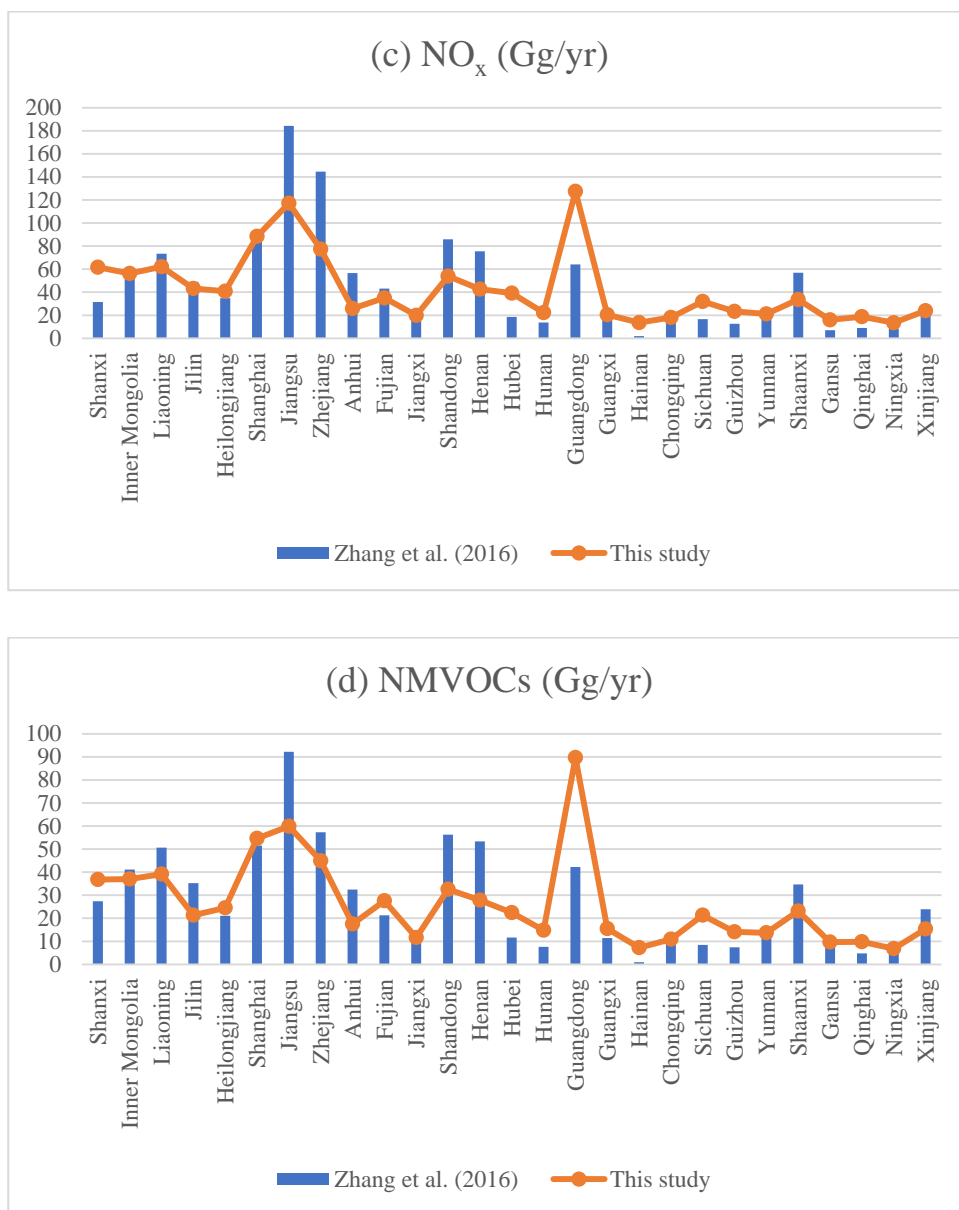


Fig. S7. Comparison of JJJ’s emissions generated by interprovincial exports with the research of Zhao *et al.* (15)

12. Comparison with the actual measures

The formation of haze in JJJ is dominated by pollutant emissions from coal combustion for power generation, metal production and non-metal production (15). Coal combustion is the main source of air pollution, accounting for 30% of JJJ’s total primary PM_{2.5}, 65% of SO₂, and 45% of NO_x (62). Electricity generation, metal production, and non-metal production contribute 9%, 15%, and 20% of primary PM_{2.5}, 22%, 8%, and 9% of SO₂, as well as 26%, 7%, and 10% of NO_x in JJJ region, respectively (62). Thus, the measures of coal consumption control, clean energy generation, and elimination of metal and non-metal industries with old technologies are incorporated in the current model to simulate air policy scenarios in JJJ region and quantify their impacts on primary PM_{2.5} and secondary precursor emissions in the target region and spillover effects to other regions. There are some other actual measures taken in JJJ including urban construction dust control and transportation-related air pollution prevention like improvement of gasoline quality and update of old vehicles. However, the construction dust pollution and traffic pollution only contribute to less than 3% and 5% of primary PM_{2.5} emissions (62), which are omitted in the JJJ air policy scenario. Table S6 illustrates the comparison of the actual and modeled JJJ emission reduction measures.

Table S6 Comparison of the actual and modeled JJJ emission reduction measures.

Sector	Actual Measures	Modeled Measures
Coal consumption	<ul style="list-style-type: none"> • Reduction of total coal consumption • Coal to electricity • Coal to gas 	<ul style="list-style-type: none"> • Beijing reduces coal consumption to 10 million tons. • Tianjin reduces coal consumption to 42 million tons. • Hebei reduces coal consumption to 260 million tons.
Electricity production and supply	<ul style="list-style-type: none"> • Clean energy generation • Importing electricity from other regions 	<ul style="list-style-type: none"> • No coal-fired power generation in Beijing. • Beijing imports 70% electricity from outside. • Tianjin imports 35% electricity from outside.
Metal production	<ul style="list-style-type: none"> • Reduction of metal production with old technologies 	<ul style="list-style-type: none"> • Tianjin reduces steel production to less than 5 million tons. • Hebei eliminates steel production by 60 million tons, and iron production by 60 million tons.
Nonmetal production	<ul style="list-style-type: none"> • Reduction of nonmetal production with old technologies 	<ul style="list-style-type: none"> • Beijing reduces cement production to 4 million tons. • Tianjin reduces cement production to less than 5 million tons • Hebei eliminates 61 million tons of cement production, and 1.8 million tons of glass production.
Construction	<ul style="list-style-type: none"> • Urban construction dust control 	<ul style="list-style-type: none"> • Omitted
Transportation	<ul style="list-style-type: none"> • Transportation-related air pollution prevention 	<ul style="list-style-type: none"> • Omitted

China Meteorological Administration reported that the PM_{2.5} of JJJ in 2017 showed an almost 39% decline from 2013, illustrating the success of the Clean Air Action

(http://www.cma.gov.cn/2011xwzx/2011xmtjj/201802/t20180201_461474.html). The scenario for air pollution mitigation developed in this study shows that the PM_{2.5} reduction is about 34%, which is close to the actual measurements.