# Probing the occurrence, sources and cancer risk assessment of polycyclic aromatic hydrocarbons in $PM_{2.5}$ in a humid metropolitan city of China

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Table S1 The general information of meteorological conditions during sampling period (The AQI and PM2.5 marked red indicate higher than associated standard).

| Date | T (℃) | RH (%) | AQI | $PM_{2.5}$ ($\mu g/m^3$) | Wind speed | Pressure |
|---|---|---|---|---|---|---|
| 2021.12.01 | 8-15 | 81 | 55 | 35 | 2m/s | 102.8kPa |
| 2021.12.02 | 8-16 | 92 | 73 | 53 | 0m/s | 102.8kPa |
| 2021.12.03 | 7-17 | 92 | 85 | 63 | 2m/s | 102.7kPa |
| 2021.12.05 | 11-17 | 90 | 115 | 87 | 1m/s | 102.7kPa |
| 2021.12.06 | 10-18 | 87 | 104 | 78 | 1m/s | 102.4kPa |
| 2021.12.07 | 11-14 | 86 | 123 | 93 | 2m/s | 102.0kPa |
| 2021.12.08 | 11-12 | 72 | 73 | 53 | 1m/s | 102.6kPa |
| 2021.12.09 | 11-14 | 88 | 103 | 81 | 1m/s | 102.5kPa |
| 2021.12.10 | 11-13 | 72 | 118 | 89 | 2m/s | 102.1kPa |
| 2021.12.11 | 10-12 | 93 | 80 | 59 | 2m/s | 102.6kPa |
| 2021.12.12 | 9-12 | 86 | 29 | 20 | 2m/s | 103.3kPa |
| 2021.12.13 | 9-15 | 93 | 44 | 30 | 2m/s | 102.6kPa |
| 2021.12.14 | 11-14 | 73 | 43 | 31 | 3m/s | 101.9kPa |
| 2021.12.15 | 11-13 | 82 | 63 | 45 | 0m/s | 101.6kPa |
| 2021.12.16 | 9-12 | 76 | 83 | 61 | 2m/s | 102.2kPa |
| 2021.12.17 | 9-10 | 74 | 44 | 27 | 2m/s | 103.1kPa |
| 2021.12.18 | 8-10 | 92 | 50 | 35 | 3m/s | 103.1kPa |
| 2021.12.19 | 6-12 | 79 | 57 | 40 | 1m/s | 102.9kPa |
| 2021.12.20 | 7-13 | 80 | 70 | 51 | 2m/s | 102.5kPa |
| 2021.12.21 | 7-13 | 92 | 77 | 56 | 2m/s | 102.5kPa |
| 2021.12.22 | 8-15 | 94 | 75 | 55 | 2m/s | 102.3kPa |
| 2021.12.23 | 7-12 | 83 | 103 | 77 | 2m/s | 101.5kPa |
| 2021.12.24 | 8-13 | 90 | 143 | 109 | 0m/s | 102.2kPa |
| 2022.1.01 | 4-13 | 91 | 139 | 95 | 1m/s | 103.2kPa |
| 2022.1.02 | 5-12 | 82 | 89 | 66 | 1m/s | 103.0kPa |

| | | | | | | |
|---|---|---|---|---|---|---|
| 2022.1.03 | 8-10 | 76 | 75 | 43 | 2m/s | 103.0kPa |
| 2022.1.05 | 6-13 | 89 | 113 | 85 | 1m/s | 99.1kPa |
| 2022.1.06 | 9-11 | 82 | 90 | 67 | 1m/s | 99.4kPa |
| 2022.1.07 | 8-10 | 71 | 79 | 58 | 0m/s | 99.5kPa |
| 2022.1.08 | 7-12 | 80 | 53 | 37 | 1m/s | 99.5kPa |
| 2022.1.09 | 6-14 | 92 | 58 | 40 | 1m/s | 99.2kPa |
| 2022.1.10 | 8-13 | 75 | 62 | 44 | 1m/s | 99.2kPa |
| 2022.1.11 | 9-15 | 83 | 78 | 57 | 0m/s | 99.4kPa |
| 2022.1.12 | 9-11 | 73 | 79 | 58 | 1m/s | 99.1kPa |
| 2022.1.13 | 8-10 | 84 | 124 | 94 | 1m/s | 99.5kPa |
| 2022.1.14 | 7-12 | 74 | 63 | 45 | 0m/s | 99.0kPa |
| 2022.1.15 | 8-12 | 74 | 69 | 50 | 1m/s | 99.3kPa |
| 2022.1.16 | 8-13 | 79 | 89 | 66 | 1m/s | 99.7kPa |
| 2022.1.17 | 5-13 | 79 | 99 | 74 | 0m/s | 99.8kPa |
| 2022.1.19 | 6-17 | 71 | 97 | 72 | 1m/s | 99.2kPa |
| 2022.1.20 | 10-12 | 77 | 102 | 76 | 0m/s | 98.4kPa |
| 2022.2.16 | 10-14 | 62 | 59 | 42 | 3m/s | 101.5kPa |
| 2022.2.17 | 8-12 | 61 | 25 | 15 | 2m/s | 98.6kPa |
| 2022.2.18 | 9-12 | 72 | 25 | 15 | 3m/s | 102.1kPa |
| 2022.2.19 | 7-8 | 90 | 32 | 20 | 2m/s | 99.8kPa |
| 2022.2.20 | 5-8 | 80 | 36 | 25 | 1m/s | 99.9kPa |
| 2022.2.21 | 4-10 | 64 | 40 | 23 | 3m/s | 100.0kPa |
| 2022.2.22 | 3-9 | 75 | 37 | 25 | 2m/s | 100.2kPa |
| 2022.2.23 | 3-12 | 52 | 44 | 28 | 2m/s | 100.1kPa |
| 2022.2.25 | 7-14 | 63 | 63 | 43 | 2m/s | 99.6kPa |
| 2022.2.26 | 8-15 | 55 | 83 | 61 | 1m/s | 99.7kPa |
| 2022.2.27 | 12.5 | 55 | 85 | 63 | 2m/s | 98.6kPa |

Table S2 The detailed human respiratory exposure parameters associated with ILCR and PAF.

| | Age (years) | IR ($m^3/d$) | BW (kg) | AT (a) | EF (d/a) | ED (a) | ET (h/d) | EFA | ASF |
|---|---|---|---|---|---|---|---|---|---|
| Children | 6-12 | 11.50±1.95 | 33.37±11.12 | 78 | 365 | 9 | 1.90±0.79 | 0.86 | 2 |
| Adolescents | 13-17 | 13.75±3.12 | 55.79±11.72 | 78 | 365 | 15 | 1.69±0.57 | 0.86 | 2 |
| Adults | 18-59 | 16.70±2.56 | 62.70±11.30 | 78 | 365 | 39 | 4.31±2.85 | 0.86 | 1 |
| Seniors | 60-80 | 13.80±1.78 | 60.30±11.19 | 78 | 365 | 70 | 4.02±2.55 | 0.86 | 1 |

The adoption of these parameters aims to align as closely as possible with the actual demographics of the sampled regions. The data for IR, BW, and ET were derived from a survey on exposure parameters conducted specifically for the Chinese population[1,2]. In the original survey report, IR, BW, and ET are only provided with their mean and quartile values. For the purpose of simulation and calculation convenience, it is assumed that they follow a normal distribution. The standard deviation is derived from a specific proportional relationship between the mean and quartile values of the normal distribution, known as the quartile pseudo-standard deviation (F-pseudosigma). Specifically, the F-pseudosigma is obtained by dividing the difference between the upper and lower quartiles by 1.349, and this value is used as the standard deviation for the dataset. AT data was obtained from the *Chongqing City Annual Resident Health Status Report 2020*, released by the Chongqing Municipal Health Commission, which can available on the web site at: https://wsjkw.cq.gov.cn/zwgk_242/wsjklymsxx/jkfw_266458/gzxx_266460/202109/t20210930_9779478.html. EFA, ASF, and Gensus are sourced from the research findings of Shen et al. focusing on Asian populations[3]. The resulting distributions of GeneSus follow log-normal distributions, and the standard variations of distributions of log10-transformed individual GeneSus for Asian 0.65.

Table S3 Limit of detection (LOD) ($pg/m^3$) and limit of quantitation (LOQ) ($pg/m^3$) for target PAHs.

| | Nap | Acy | Ace | Flu | Phe | Ant | Flt | Pyr | BaA | Chr | BbF | BkF | BaP | IcdP | DBA | BghiP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| LOD | 0.27 | 0.09 | 0.21 | 0.01 | 0.39 | 0.39 | 0.01 | 0.01 | 0.01 | 0.37 | 0.22 | 1.26 | 0.93 | 0.16 | 0.06 | 0.06 |
| LOQ | 0.89 | 0.29 | 0.70 | 0.15 | 1.29 | 1.29 | 0.05 | 0.04 | 0.03 | 1.23 | 0.75 | 4.19 | 3.11 | 0.54 | 0.19 | 0.19 |

Table S4 Recovery of surrogate standard in procedure blank and method blank samples.

| surrogate standard | procedural blank | method blank |
|---|---|---|
| Nap-d8 | 68.6 | 84.4% |
| Ace-d10 | 75.8% | 85.8% |
| Phe-d10 | 89.7% | 106.7% |
| Chr-d12 | 95.7% | 108.3% |
| Per-d12 | 101.8% | 97.6% |

Table S5 The concentrations of 16 PAHs ($ng/m^3$) in all $PM_{2.5}$ samples (average, min to max).

| **Species** | **2021,12（n=23）** | **2022,01（n=18）** | **2022,02（n=11）** | **Average** |
|---|---|---|---|---|
| Nap | 28.34（12.35-81.30） | 17.55（6.20-31.00） | 12.71（4.20-19.45） | 19.53 |
| Ac | 0.17（0.10-0.25） | 0.15（0.10-0.20） | 0.11（0.05-0.20） | 0.14 |
| Ace | 0.19（0.05-0.30） | 0.12（0.05-0.25） | 0.13（0.05-0.35） | 0.15 |
| Fl | 0.30（0.10-0.80） | 0.26（0.10-0.75） | 0.22（0.10-0.60） | 0.26 |
| Phe | 2.00（0.90-3.95） | 1.92（1.05-3.70） | 1.58（0.75-3.80） | 1.83 |
| Ant | 0.44（0.10-2.20） | 0.16（0.10-0.25） | 0.57（0.05-3.70） | 0.39 |
| 2-3 ring | 31.44（13.65-88.85） | 20.15（7.50-36.15） | 15.32（5.20-28.10） | 22.30 |
| Flu | 3.89（2.05-6.15） | 4.10（2.40-5.60） | 2.54（1.00-4.30） | 3.51 |
| Pyr | 4.00（2.15-6.35） | 4.00（2.50-5.30） | 2.49（1.25-4.00） | 3.50 |
| BaA | 1.84（0.60-6.70） | 1.61（0.80-2.40） | 0.72（0.30-1.50） | 1.39 |
| Chr | 6.74（2.65-13.15） | 7.04（3.95-10.45） | 3.34（1.90-5.15） | 5.71 |
| 4 ring | 16.47（7.45-32.40） | 16.76（9.60-23.75） | 9.10（4.45-14.95） | 14.11 |
| BbF | 9.60（4.80-16.50） | 9.11（4.75-13.4） | 3.77（2.30-6.80） | 7.49 |

| | | | | |
|---|---|---|---|---|
| BkF | 2.64（1.05-4.70） | 2.62（1.50-3.75） | 1.20（0.65-1.80） | 2.15 |
| BaP | 4.22（1.65-8.25） | 3.93（2.20-5.60） | 1.57（0.95-2.70） | 3.24 |
| IP | 5.21（2.50-9.40） | 5.10（2.85-7.40） | 2.19（1.30-3.55） | 4.17 |
| DBA | 1.78（0.65-3.15） | 1.69（0.80-2.70） | 0.50（0.05-0.85） | 1.32 |
| BghiP | 5.99（2.80-10.95） | 5.38（2.95-7.55） | 2.28（1.55-3.15） | 4.55 |
| 5-6 ring | 29.43（13.50-52.90） | 27.83（15.10-40.40） | 11.51（6.80-18.85） | 22.92 |
| 16PAHs | 77.34（34.60-174.15） | 64.74（32.20-100.30） | 35.93（16.45-61.40） | 59.32 |

Table S6 Comparison of PAHs Concentrations in $PM_{2.5}$ or total suspended particulate matter (TSP) across different sampling regions.

| Sampling site | Sampling time | Species | Sample type | Concentration | Reference |
|---|---|---|---|---|---|
| Chongqing | Winter 2021 | 16PAHs | TSP | 59.35 | This study |
| Beijing | Winter 2013 | 16PAHs | TSP | 120.20 | [4] |
| Nanjing, Jiangsu | Winter 2014 | 18PAHs | TSP | 50.60 | [5] |
| Wuhan, Hubei | Winter 2011 | 16PAHs | TSP | 59.77 | [6] |
| Chengdu, Sichuan | Winter 2010 | 16PAHs | TSP | 71.38 | [7] |
| Nanchang, Jiangxi | Winter 2014 | 15PAHs | TSP | 22.54 | [8] |
| Shanghai | Winter 2014 | 16PAHs | TSP | 15.90 | [9] |
| Hong Kong | Winter 2011 | 16PAHs | TSP | 4.60 | [10] |
| Guangzhou, Guangdong | Winter 2016 | 16PAHs | TSP | 10.31 | [11] |
| Hangzhou, Zhejiang | Winter 2021 | 16PAHs | PM2.5 | 27.90 | [12] |
| Jinan, Shandong | Winter 2016 | 16PAHs | PM2.5 | 72.60 | [13] |
| Harbin, Heilongjiang | Winter 2008 | 16PAHs | TSP | 85.70 | [14] |
| Kunming, Yunnan | Winter 2012 | 16PAHs | TSP | 46.89 | [15] |
| Guiyang, Guizhou | Winter 2005 | 16PAHs | TSP | 18.40 | [16] |
| Xi’an, Shaanxi | Winter 2016 | 16PAHs | PM2.5 | 115.00 | [17] |
| Zhengzhou, Henan | Winter 2018 | 16PAHs | PM2.5 | 45.80 | [18] |
| Taiyuan, Shanxi | Winter 2012 | 16PAHs | PM2.5 | 215.93 | [19] |

Table S7 The comparison of 16PAHs between normal and polluted days during sampling period.

| PAHs | 2021, 12 | | 2022, 01 | |
|---|---|---|---|---|
| Species | Polluted days | Normal days | Polluted days | Normal days |
| Nap | 26.45 | 19.95 | 18.00 | 13.20 |
| Acy | 0.20 | 0.15 | 0.15 | 0.10 |
| Ace | 0.20 | 0.15 | 0.10 | 0.10 |
| Flu | 0.35 | 0.30 | 0.35 | 0.20 |
| Phe | 2.35 | 1.70 | 2.30 | 1.50 |
| Ant | 0.45 | 0.10 | 0.15 | 1.50 |
| Flt | 4.75 | 2.70 | 4.45 | 3.05 |
| Pyr | 4.85 | 2.70 | 4.30 | 2.95 |
| BaA | 2.10 | 0.85 | 1.65 | 1.15 |
| Chr | 1.73 | 3.95 | 7.70 | 5.00 |
| BbF | 8.65 | 5.50 | 10.05 | 6.70 |
| BkF | 3.40 | 1.55 | 2.90 | 1.90 |
| BaP | 5.50 | 2.20 | 3.90 | 2.90 |
| IcdP | 6.90 | 3.05 | 5.45 | 3.65 |
| DBA | 2.15 | 0.9 | 1.75 | 1.15 |
| BghiP | 7.80 | 3.4 | 5.55 | 3.00 |
| $\sum_{16}$PAHs | 88.35 | 49.1 | 68.85 | 47.55 |

Table S8 Comparison of the recorded annual lung cancer incidence rates with the modeled lung cancer risk due to ambient PAHs exposure.

| Age groups (y) | Actual incidence rate of lung cancer in Chongqing in 2017 ($\times 10^{-5}$) | Model predicted PAF (%) | | Model predicted excess annual lung cancer incidence rate by PAF approach ($\times 10^{-6}$) | | Model predicted ILCR ($\times 10^{-6}$) | |
|---|---|---|---|---|---|---|---|
| | | URR=4.49 | URR=1.3 | URR=4.49 | URR=1.3 | | ET=24h |
| 6-12 | —— | 2.31 | 0.44 | —— | —— | 0.25 | —— |
| 13-18 | —— | 2.05 | 0.38 | —— | —— | 0.23 | —— |
| 19-60 | 245.82 | 1.08 | 0.19 | 26.54 | 4.67 | 0.71 | 4.31 |
| 61-80 | 348.29 | 1.08 | 0.20 | 37.62 | 6.96 | 1.23 | 7.03 |

Table S9 Total toxic equivalent (TEQ) and excess incremental lifetime carcinogenic risk (ILCR) of PAHs in different cities (ND- Not Detected).

| Location/Country | Sampling period | PAHs Species | ∑PAHs (ng/m$^3$) | TEQ (ng/m$^3$) | ILCR | | References |
|---|---|---|---|---|---|---|---|
| | | | | | Children (×10$^{-6}$) | Adults (×10$^{-6}$) | |
| Chongqing, China | 2021-2022 | 16 | 59.35 | 6.23 | 0.53 | 2.45 | This study |
| Nanjing, China | 2015 | 16 | 91.80 | 1.09 | 0.26 | 0.41 | [20] |
| Dongguan, China | 2017-2018 | 16 | 40.27 | ND | 3.81 | 4.83 | [21] |
| Shenzhen, China | 2012-2013 | 16 | 111.90 | 2.44 | 0.20 | 1.23 | [22] |
| Xi'an, China | 2013 | 16 | 57.10 | 6.90 | ND | 7.60 | [23] |
| Jamshedpur, India | 2018-2019 | 16 | 321.71 | 69.39 | 12.71 | 30.53 | [24] |
| Agra, India | 2010-2012 | 16 | 1668.10 | 37.10 | 4.19 | 99.80 | [25] |
| Tehran, Iran | 2018-2019 | 16 | 20.10 | 2.92 | ND | 3.14 | [26] |

## Text S1 Air mass back trajectories

Frequencies of the 72-hour air mass back trajectories arriving at sampling site during the sampling period are shown as percentages in Figure S1 and show source regions may extend as far as Henan in northern China and Myanmar bordering Yunnan Province. However, in general, air masses typically derived from north and east regions near to Chongqing as air masses in winter were affected by temperature and terrain, making the transport speed slow and paths relatively short. From Figure S1 it can be seen that the air parcels arriving during December 2021 mainly came from Sichuan Province and eastern Chongqing, accounting for 38.7% and 21.7%, respectively. In January 2022 air masses mainly came from eastern and southeast Chongqing (36.9% and 22.7%, respectively) while in February 2022 air masses mainly came from southwest Chongqing, Hubei Province and Hunan Province, accounting for 24.7%, 33.3% and 21.9%, respectively.

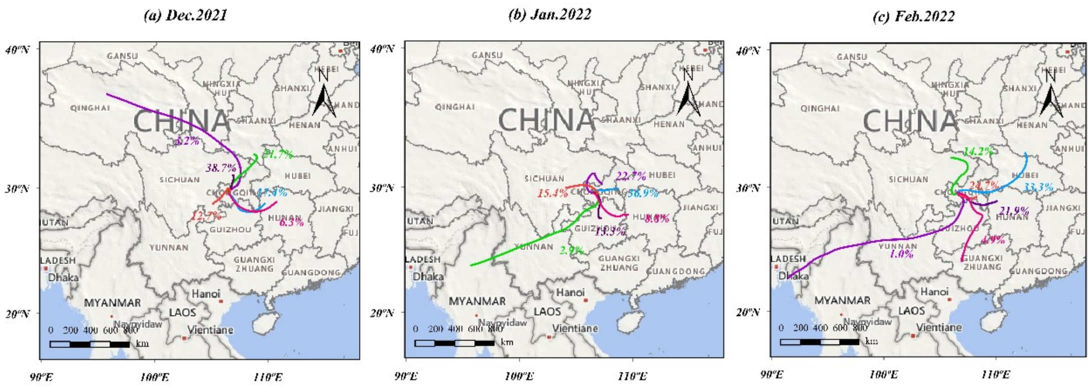


Figure S1 Frequencies of the 72-hour air mass back trajectories arriving at sampling site during the sampling period.

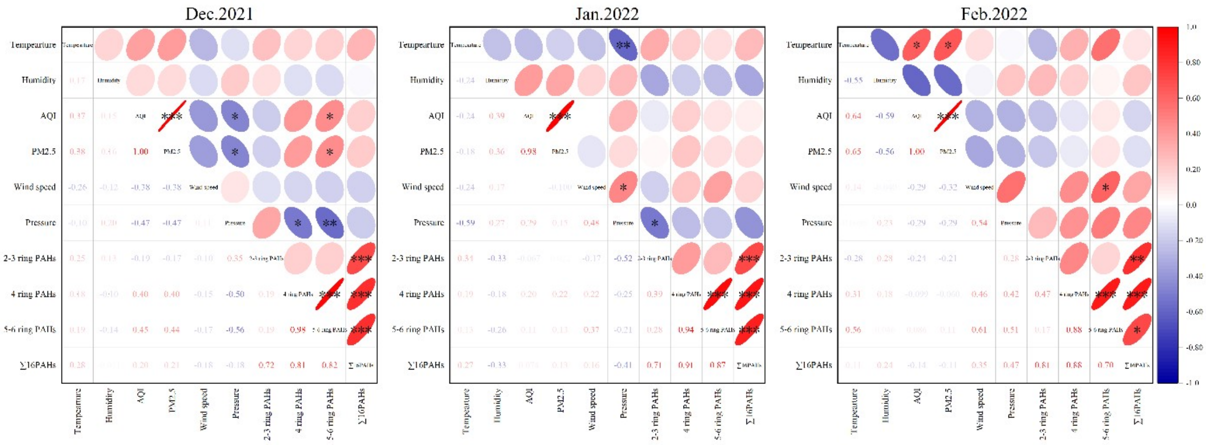


Figure S2 The correlations between the 16 PAHs and six parameters, including temperature, relative humidity, wind speed, air pressure, air quality index (AQI) and concentration of $PM_{2.5}$ (* p<=0.05    ** p<=0.01    *** p<=0.001).

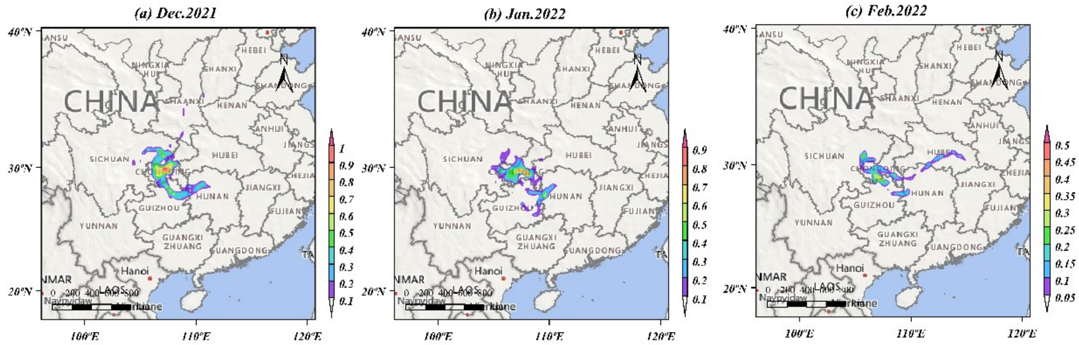


Figure S3 The potential sources of PAHs by PSCF algorithm during the sampling period.

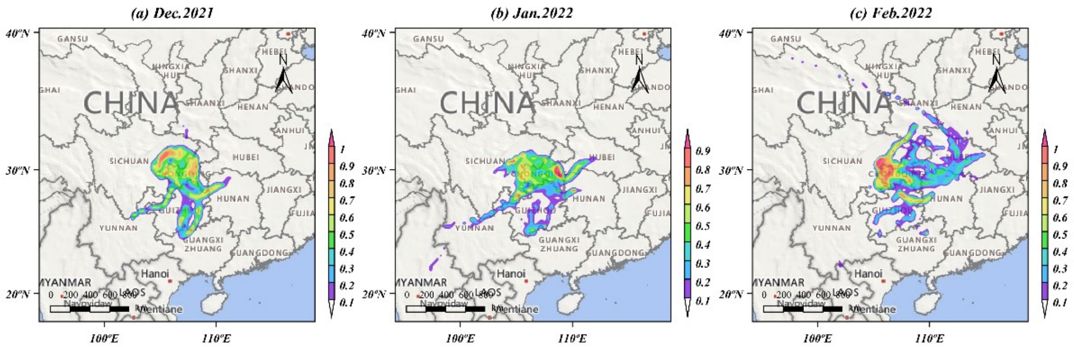


Figure S4 The potential sources of $PM_{2.5}$ concentrations by PSCF algorithm during the sampling period.

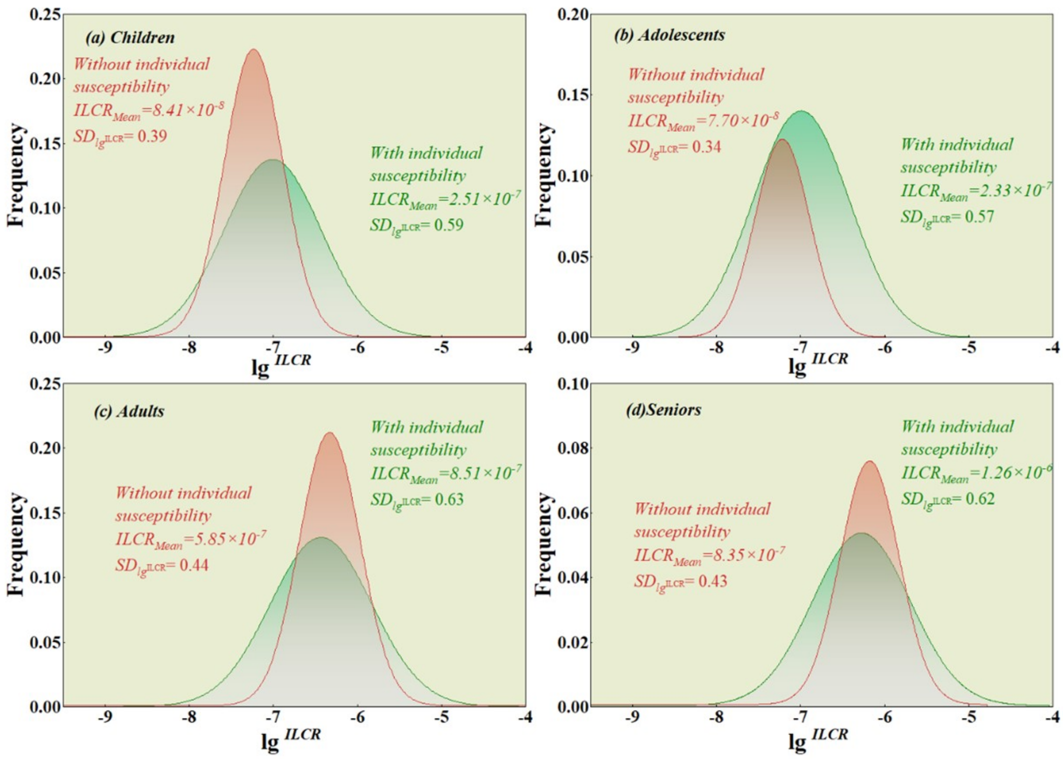


Figure S5 Probability distribution of ILCR simulation results considering overall susceptibility and without overall susceptibility.

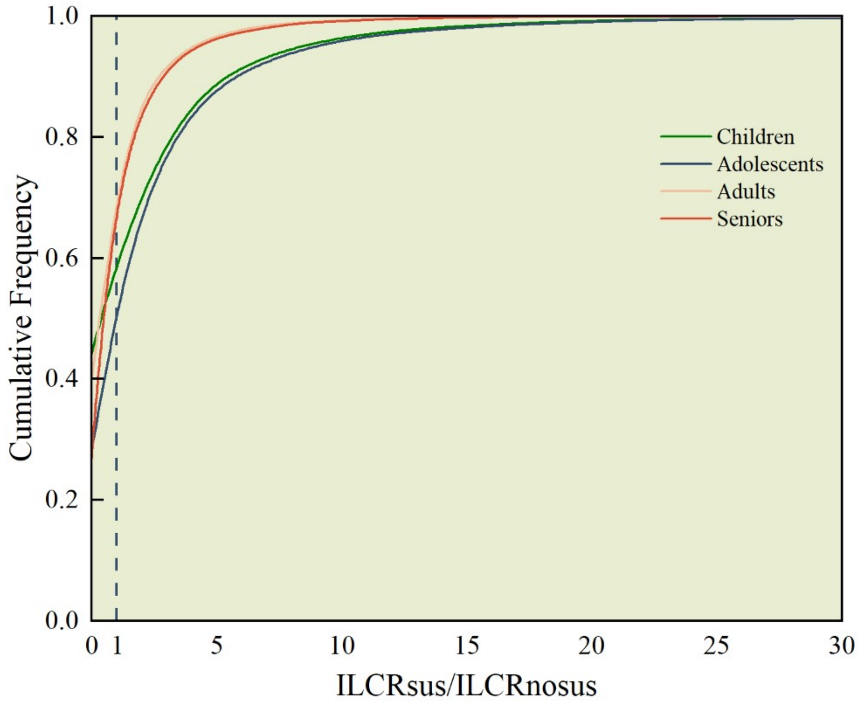


Figure S6 Cumulative curves of ILCR rate distribution results from 10,000 Monte Carlo simulations with and without considering individual susceptibility.

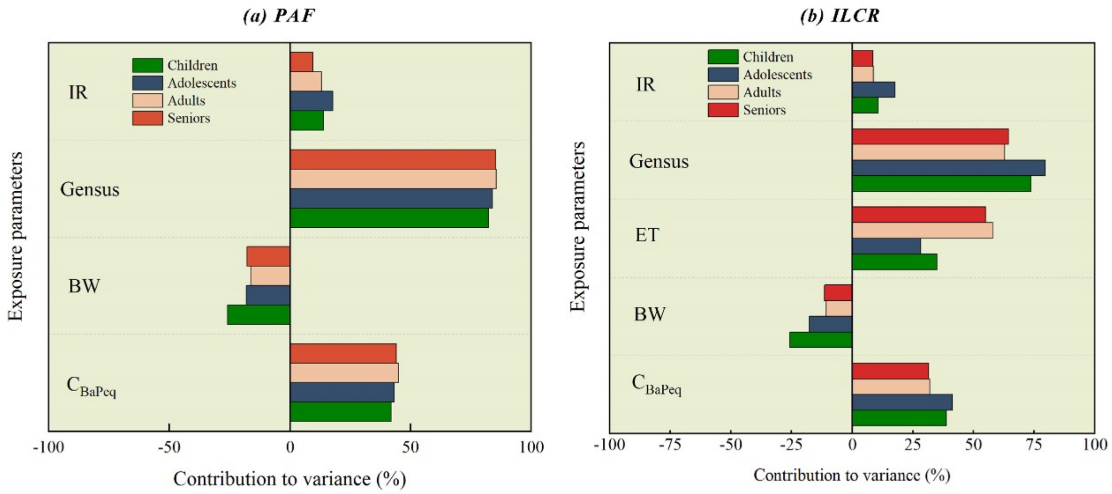


Figure S7 Sensitivity analysis results for PAF (a) and ILCR (b) models.

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