ENVIRONMENTAL DISTRIBUTIONS OF BENZO[a]PYRENE (BaP) IN CHINA: CURRENT AND FUTURE EMISSION REDUCTION SCENARIOS EXPLORED USING A SPATIALLY EXPLICIT MULTI-MEDIA FATE MODEL

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Abstract

SESAMe v3.0, a spatially resolved multi-media fate model with 50 × 50 km² resolution, has been developed for China to predict environmental concentrations of Benzo(a)pyrene (BaP) using an atmospheric emission inventory for 2007. Model predictions are compared with environmental monitoring data obtained from an extensive review of the literature. The model performs well in predicting multi-media concentrations and distributions. Predicted concentrations are compared with guideline values; highest values with some exceedances occur mainly in the North China Plain, Mid Inner Mongolia, and parts of three northeast provinces, Xi’an, Shanghai and south of Jiangsu province, East Sichuan Basin, middle of Guizhou and Guangzhou. Two potential future scenarios have been assessed using SESAMe v3.0 for 2030 as BaP emission is reduced by 1) technological improvement for coal consumption in energy production and industry sectors in Scenario 1 (Sc1); and 2) technological improvement and control of indoor biomass burning for cooking and indoor space heating, and prohibition of open burning of biomass in 2030 in Scenario 2 (Sc2). Sc2 is more efficient in reducing the areas with exceedance of guideline values. Use of SESAMe v3.0 provides insights on future research needs and can inform decision-making on options for source reduction.

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**Introduction**

Polycyclic aromatic hydrocarbons (PAHs) inputs into the environment are largely derived from inefficient combustion processes and several are known mutagens/carcinogens. They are of environmental and public health concern, so many countries have developed environmental emission and quality criteria. They are also the subject of international agreements and concern due to their long-range atmospheric transport potential. While emissions and atmospheric concentrations have been declining in some developed countries, global emissions inventories show shifts in primary emissions to rapidly developing countries, where inefficient fossil fuel combustion for power generation, metal production and other industrial processes, along with transport, waste incineration and biomass burning are often major sources. China is now a key part of the global inventory – constituting an estimated 20% of the global emissions in 2007. It is therefore particularly important to understand/confirm the key sources in China, where they are distributed and how efforts at control may affect contemporary and future environmental concentrations.

Benzo(a)pyrene (BaP) is a carcinogenic high molecular weight PAH which is emitted to atmosphere on fine particulates (PM10 and 2.5) and often associated with black carbon (BC). The estimated emission of BaP across China in 2007 was ~1100 tonnes. However, spatial resolution is important for China, a country of >1.3 billion people, because the population, industrial development, PAH sources and environmental features vary widely. BaP is one of the most studied compounds in China, with many papers reporting on PAHs in the environment. This makes it an ideal choice as a test chemical when exploring the links between sources and environmental levels with a multi-media environmental fate model. Other studies have previously focussed on assessing human exposure to airborne PAHs via inhalation and the distribution and ecological risk of waterborne PAHs in 7 major river basins by collecting measured data from literature. China has also recently released a ‘National Soil Pollution Gazette’ reporting on a countrywide soil pollution survey. This survey may result in new legislation that addresses soil protection for China. However, despite there now being: i. specific source inventory information; ii. a prevalence of air, water and soil data; iii. Chinese national standards for BaP in air, water and soils; iv. commitments made to reduce and regulate emissions of particulate matter and other air...
pollutants by the State Council of China (SCC) five-year ‘Action Plan for Air Pollution Control’, there has been little attempt to integrate this information with multi-media modelling tools or to assess the potential impacts of sources and their controls on ambient levels and – ultimately – for risk management. That is therefore the purpose of this paper.

Previous multimedia models developed by other researchers have not been parameterized with fine enough spatial resolution for China, nor at a national scale. As a result, we have developed SESAMe v3.0, a spatially explicit multi-media fate model which has been specifically parameterised for whole of mainland China with $50 \times 50$ km$^2$ resolution. Initially the model uses spatially resolved BaP atmospheric source inventory information for 2007 to generate model predictions to compare with environmental monitoring data obtained from the literature over the period 1997 to 2011. Quantification of the transfer of BaP between media is briefly discussed in relation to atmospheric transport, key storage media, ambient distributions etc. Based on the good model performance, predicted high background regions are identified across the country by comparing predicted ambient BaP levels with guideline values made for air, freshwater and soils. We then move on to explore two possible future scenarios where emission from coal and biomass burning are controlled and reduced by 2030 and making comparisons with the base year 2007. This is important, given the opportunity in China for large scale state intervention and control of sources (e.g. power stations; waste incinerators; vehicles), as well as changing patterns of individual behaviour on the consumption of biofuels. SESAMe v3.0 has been used to assess the efficiency of emission reduction in the two scenarios. Our purpose is to show how multimedia models such as SESAMe v3.0 could be used to make informed decisions about possible source control options.

**Materials and Methods**

**Model definition**

SESAMe v3.0 is an improved version of the previously described SESAMe model and equations for transport processes are taken from Simplebox 3.24a and MAMI III models; it has a higher spatial resolution than SESAMe with 5468 independent $50 \times 50$ km$^2$ grid cells that cover mainland China and is therefore similar in structure to ChemCan and CHEMFRANCE. Each grid cell represents a region, which is surrounded by 8 adjacent $50 \times 50$ km$^2$ grid cells that constitute a movable continental scale; the regional scale and the continental scale are connected by non-directional advective flow exchange, and so the model doesn’t directly simulate how BaP is transported from one grid cell to another (details see Supporting Information (SI) and Figure S1). This structure, therefore, considers the influence of the emission and environmental processes of the surrounding region to each cell, which is
in contrast to ChemCan and CHEMFRANCE. Further improvements have been made for this study, including: the addition of sea water compartments, referring to Simplebox 3.24a\textsuperscript{32} spatial data layers for soil density,\textsuperscript{35} soil pH\textsuperscript{35} and aerosol contents in air; the consideration of the temperature effect on degradation rates, referring to Simplebox 3.24a\textsuperscript{32} (SI) and the inclusion of agricultural soil irrigation by surface freshwater to ensure environmental processes in the model more complete. For the agricultural soil irrigation, this version of the model assumes that ~370 billion m\textsuperscript{3} water was consumed in the whole country for irrigation\textsuperscript{36} and distributed uniformly to agricultural soil across the country, and that the irrigation water in each grid cell originated from local freshwater sources in the same grid cell. Each grid cell has compartments describing air, freshwater and sediment, sea water and sediment, natural soil (defined as forest land, grassland, desert, wetland and all the other unused land), agricultural soil (cropland soil), urban soil (rural residential land was included), natural vegetation (on natural soil) and agricultural vegetation (on agricultural soil). There are 65 environmental parameters for each grid cell, in which 47 are fixed default values for all regions and 18 are spatially variable (Table S1 and S2 in SI); the chemical parameters of BaP are given in Table S3.

\textbf{Emission inventory}

The BaP emission dataset for the year 2007 used in this study originated from Shen et al.\textsuperscript{10} From their study, it was estimated that the emission of BaP in 2007 for the whole of mainland China (exclusive of Taiwan and Hainan islands) was approximately 1032 tonnes. Nationally, the major BaP sources in China are indoor biomass burning (43\%, firewood and crop residue), coke production (21\%) and primary Al production (12\%); the domestic coal burning is about 13\%; motor vehicle emissions only constituted an estimated 2\% and open fire agriculture waste burning 1.2\%.\textsuperscript{10} However, the dominant sources vary geographically as a complex function of industrial activity, urbanization level, living standards, climate and policies across China. For example, indoor biomass burning is an important source in large areas of the North China Plain (NCP), Yangtze River Delta (YRD), Anhui, Hubei, Sichuan and the northeast provinces etc.; coal consumed in coke production is a major source in Shanxi and Inner Mongolia (Ordos); vehicle diesel is an important source for Shanghai and parts of Beijing.\textsuperscript{10} Sources were aggregated in the 50 × 50 km\textsuperscript{2} grid, as detailed in SI, with the national distribution shown in Figure 4a.

\textbf{Model evaluation}

Emissions for the base year of 2007 were run to steady state to generate predicted BaP environmental concentrations, which could be compared with measured data and the environmental guideline values/quality standards. The following guideline values were used:
ambient air quality values of 1 ng/m³ as an annual average and 2.5 ng/m³ as a daily average;¹⁰
soil values of 100 ng/g taken from the ‘Technical regulations for national soil contamination
assessment’ for Chinese soil pollution survey for soil pollution identification, to compare
with the results in the ‘National Soil Pollution Gazette’; freshwater guideline values of 2.8
ng/L from Chinese standards²⁰ and 15 ng/L from Canadian standards.³⁸

To evaluate the model, hundreds of peer-reviewed papers on BaP occurrence in China were
found. BaP concentration data were compiled without any filter for environmental media
from ca. 130 peer-reviewed literature sources where sampling site location information was
given. Focus was on the sampling years 1997-2011 and proximity to the 2007 base emission
year (Table S4). Figure 1 shows the location of the measurement data used for air, freshwater,
freshwater sediment and soil. When several sampling sites fall into the same grid cell (Figure
1b), the mean measured value was taken to compare with the predicted concentration in that
grid cell.

The dimensions of the selected continental and regional scales within the current model
structure are believed to be suitable to capture the majority of the emissions considering the
transport distance of BaP is probably a few hundreds of kilometres. However, to ensure that
the selected spatial scale is appropriate for BaP, it was compared with two previous versions
of the model which have different spatial scales and grid cell dimensions (more details see SI).

Figure 1. a, sampling sites of observed data taken from the literature across China; b,
illustrating the 50 × 50 km² grid covering North China Plain and Bohai Bay in the model and
the overlay of sampling sites and model grid.

The uncertainty of SESAMe v3.0 was explored by Monte Carlo simulation (details see SI).
The BaP concentration in 10 media was calculated 10,000 times. Normal and lognormal
distributions were assessed according to the probability distribution of different input parameters. Values for the emission vector and the 18 environmental variable vectors were randomly produced based on their probability distributions. A variability-based sensitivity coefficient (SCV, see S1) was applied to the sensitivity analysis, considering the coefficient of variation of the 18 spatially variable parameters for identifying influential parameters. The parameters with an SCV index > 0.1 were identified as most influential to the model output.

**Model evaluation and discussion of results**

Figure 2. a. Comparison of predicted (all predicted data) and measured BaP concentrations in each compartment across China; b-e. point-to-point comparison of BaP concentrations in natural soil, air, freshwater and sediment (only predicted data with corresponding measured data was used); the blue lines in c-d are BaP guideline values for air (1 ng/m$^3$) and freshwater (1.5e+4 ng/m$^3$)

This version of SESAMe predicts regional or countrywide ‘background’ concentrations. Such models do not identify hotspots, but predict the regional/grid cell averaged background levels. Figure 2a presents a comparison of predicted and measured BaP concentrations for each modelled environmental compartment. Generally, the agreement across all media is good, with the model capturing the range and actual concentrations very effectively. Most points fall within the 1:10 line, with many clustered around the 1:1 line (Figure 2b-e and Figure S4), which indicates that model performance is better for freshwater, sediment and soil than that...
shown by Simplebox 3.0, EVn-BETR and IMPACT2002 in the study by Armitage et al. The selected dimensions of the regional and continental scales are important for models of this type. The selected grid dimensions in SESAME v3.0 provide improved agreement with the measurement data compared to two previous versions of the model with different grid dimensions for regional and continental scales (SI). Figure 2a suggests that slightly systematic under-prediction appears for several media but not for background concentrations. Often the measured data collected from the literature highlights industrial parks or cities, agricultural soil irrigated by wastewater, locations where dense coal burning for heating takes place, urban areas with intensive transportation and so on, e.g. those points falling below the lower 1:10 line. This may cause the underestimation shown in Figure 2a, but the model actually reflects the average situation in each grid cell. As precipitation is assumed to be continuous in the model, it is most likely to overestimate deposition rates for BaP, leading to the underestimation of air concentrations in some regions. However, this effect appears to be limited at a national scale. The distribution of BaP concentrations in different media is log-normal and the interquartile range can be found in SI Figure S3 obtained from the Monte Carlo simulation.

**BaP transport and partitioning between media:** The model predicts that after being released to the atmosphere, BaP is mainly transported to soils, water and vegetation by wet and dry deposition of particle-bound BaP; from water to sediment by sedimentation and absorption; from vegetation to soils by litter production; and from soils to water by runoff (see Figure S5-S6). The reverse processes - volatilization to air, desorption and re-suspension from sediments and transpiration are relatively unimportant. Higher precipitation rates increase the particle-bound BaP flux scavenged from air to soil or water. Areas with high soil organic matter (e.g. northeast in Heilongjiang Province) will have greater storage and retention of BaP. BaP reaches above ground vegetation primarily via particle-bound deposition, rather than from soils – in agreement with measured and other modelling studies.
Soil is the primary sink for BaP in China; at steady state 99% of BaP will be found in soil. The model defines different soil land use categories and so nationally the loadings are ~56% in agricultural soils, 35% in natural soils and 8% in urban soils. Obviously there are major regional differences, for example, with most in natural soils in the Qinghai-Tibet plateau, most in agricultural soils in NCP and Jiangsu and urban soils in Shanghai (Figure 3). For some coastal or inland catchment regions, most BaP is found in sediments (Figure 3d). Storage in sediments is only significant for the mass balance in the coastal or freshwater catchment regions. The SCV index in Table S5 shows that the BaP concentration in a region can be affected by the emission and some environmental parameters in surrounding regions. Some grid cells are more influenced by emission and transport processes in nearby areas than those within its own cell.
Figure 4. a. BaP emission; \(^{10}\) predicted BaP backgrounds levels in air (b) and freshwater (c); n in c - no freshwater

The spatial distribution of BaP: The model predicts a range of regional background concentrations (5\(^{th}\) - 95\(^{th}\) percentiles, plus median) in the different media - as follows: air, 0.002-4.6 ng/m\(^3\) (median, 0.4 ng/m\(^3\)); soils, 0.002-51 ng/g for natural soil (0.9 ng/g) and 0.05/0.06 - 56/58 ng/g for agricultural/urban soil (6.4 ng/g); fresh and sea water, 0.002-60 (4) ng/L and 1.5-11 (3.5) ng/L; fresh and marine sediments, 0.002-60 (4) ng/g and 1.5-11 (3.5) ng/L; vegetation, 0.0003-4 ng/g (0.1 ng/g) and 0.001-1.8 ng/g (0.2 ng/g) in natural and agricultural vegetation (Figure 3-4 and Figure S7-S8).

The predicted geographic distribution pattern is generally similar for air, soils and vegetation and the emission distribution pattern at the national scale (Figure 3-4). Air, soil and vegetation concentrations are generally predicted to be higher in areas such as NCP, Mid Inner Mongolia (Baotou, Ordos and Hohhot), part of the three northeast provinces (middle of Liaoning and Jilin provinces and south Heilongjiang), Xi’an in Shaanxi province, Shanghai and south of Jiangsu province, East Sichuan Basin, middle of Guizhou, Guangzhou in Guangdong province. However, environmental conditions can produce contrasting regional air and soils backgrounds. For example, a region in south Hebei has the same air concentration but nearly three times the concentration of BaP in soil compared to a region in west Inner Mongolia (Baotou). As the emission in the region of south Hebei is much higher and with higher precipitation rates in NCP compared to Inner Mongolia, more BaP is transferred to soils after being released to the atmosphere. Another interesting contrasting region in Liaoning in northeast China exhibits high soil levels close to that in another region in north Tianjin, but the air concentration is only half of that in the region in Tianjin. Runoff is similar in the two regions but the higher soil OC contents in Liaoning enhance BaP retention by soil. For most of these areas, the high background concentrations are caused mainly by indoor biomass burning (crop residue and firewood); in contrast, in Inner Mongolia, middle of Guizhou, Xi’an, some areas in Shanxi, Hebei and Shandong province in NCP, coal consumed by industry is also a key source.
Primarily BaP emissions reach aquatic systems via deposition and soil runoff. The geographic distribution in freshwater and sediment viewed at the country scale is similar to that in air and soil. However, regional differences are apparent, caused by variation in the discharge volume of rivers, runoff, and soil OC, etc. For example, BaP concentrations are extremely low in Shanghai, south Jiangsu province (22 ng/L in freshwater, 35 ng/g in sediment) in the lower reaches of the Yangtze River and the lower reaches of Yellow River (20 ng/L in freshwater, 31 ng/g in sediment) in NCP, but the air and soil concentrations in the two regions are relatively high. A region with predicted high water concentrations (173 ng/L) in the northern boundary of Anhui province has a moderate predicted BaP level in soil (68 ng/g), because the soil OC contents are lower here and runoff can transfer more BaP from soil to water, but the water discharge volume is also low.

Large areas in western China (e.g. Qinghai-Tibet plateau, large areas of Xinjiang) have lower predicted median BaP values. They are generally in the order of 0.04 ng/m$^3$ in air, 0.06 ng/g in natural soil, 0.32 ng/g in agricultural and urban soil, 0.06 ng/L in freshwater, 0.1 ng/g in sediment, and ca. 0.006 ng/g in natural and agricultural vegetation.

**Comparison of regional values and suggested guideline values for different media**

The previous sections show that the model performs well in predicting environmental concentrations. Air, soil, and freshwater are important media for public health and as noted earlier, have guideline values suggested in China and elsewhere. For air, 2.5 ng/m$^3$ has been proposed as a daily average standard. The model predicts that this is exceeded in ca. 13% of mainland China (e.g. NCP, three northeast provinces, Shanxi, north Ningxia, mid Inner Mongolia, YRD, east Sichuan, mid Guizhou, Pearl River Delta (PRD), southeast Guangxi etc.). A value of 1 ng/m$^3$ has been proposed as an annual average. This is exceeded in ca. 32% areas of mainland China (e.g. additional areas such as north and west of Guangxi, south Ningxia, south Gansu, Hunan and coastal areas in Fujian province). This exceedance ratio is close to 30% obtained in another Chinese study using the model CanMETOP which used a 1 km$^2$ spatial resolution. For soils, 100 ng/g has been adopted as a guideline value for all soils in ‘Technical regulations for national soil contamination assessment’ for national soil pollution survey. This is predicted to be exceeded in ca. 0.25% of mainland China. In contrast, this is exceeded by 1.4% of the sampling sites across China in ‘National Soil Pollution Gazette’, which reports the result of national soil pollution survey, probably because it is indicated in the Gazette that many samples were taken from seriously contaminated land. 100 ng/g is also proposed as the Chinese soil quality standard value for agricultural soil. The model predicts that it is exceeded by ca. 0.8% (about 22 thousand km$^2$) agricultural soil. These regions are mainly in Shanghai, south Jiangsu, Tianjin, and Liaoning (Shenyang and Liaoyang). For freshwater, 15 ng/L has been proposed as the Canadian guideline value. It is
exceeded by ca. 13% (ca. 20 thousand km²) of freshwater in mainland China (e.g. NCP, northeast China provinces, Shaanxi, Guizhou and east Sichuan). A value of 2.8 ng/L is proposed as the Chinese standard value. It is exceeded in ca. 40% (ca. 69 thousand km²) of freshwater (covering almost half mainland China in the east). The overestimation of median or low concentrations (blue area in Figure 2c-d) and the underestimation of high concentrations (green area in Figure 2c-d) may cause a small but acceptable bias of exceedance rates estimation but demonstrates good performance of the model.

Future scenario selection

In this section we illustrate how the model can be used to investigate the efficiency of source reduction/controls. Two scenarios are used to generate possible future ambient concentrations for the nominal year 2030.

The State Council of China (SCC) has made a five-year ‘Action Plan for Air Pollution Control’. This refers to: controlling current major industrial emissions (e.g. by improved combustion and stack controls); reducing the usage of and dependence on coal, particularly in the Beijing-Tianjin-Hebei region, the Yangtze River Delta and the Pearl River Delta; expediting the use of clean energy; controlling the number of vehicles or encouraging electric vehicles and so on. Control measures that could be most relevant to BaP emissions relate to the use of coal in industry and energy production.

Future scenario 1 (Sc 1): This considers control of coal consumption in two sectors (centralised energy production and major industrial sources). The following assumptions and principles were used to develop this scenario:

1. Coal consumption itself was not changed (2007 and 2030 levels assumed to be the same), as it’s unrealistic to foresee a reduction in coal usage in 2030 considering that the coal consumption/production in China has risen by ca. 48% from 2007 to 2012 and may currently be higher with many researchers arguing that coal consumption is likely to remain high and key to China’s economic growth. However, an action plan was developed in 2013 to reduce the coal usage in certain regions and the percentage of coal consumption in total energy consumption in China declined ca. 6% from 2007 to 2012.

2. The emissions from key sources were assumed to be reduced between 2007 and 2030 by improvements in technology and combustion conditions. (see Table 1 for details);

3. The fraction of uncontrolled and controlled activities was calculated by assuming improved technologies are introduced as described by Bond et al. in their projections about future Black Carbon emission scenarios. Controlled coal boilers
were assumed to increase from 70% to 98% for energy production and from 46% to 87% for industry (see SI for further details and Table 1); 4. Emission factors (EFs) were assumed stable over time for uncontrolled sources, while improved EFs were employed for the controlled sources. These were derived from Shen et al., with average values from their report being given in Table 1. 5. The technology improvement in the energy and industry sectors was presumed to be performed in the regions of China where coal consumption in the two sectors were > 50% to all sources, or in the regions with air backgrounds > 1 ng/m³.

Future scenario 2 (Sc 2): This scenario considered indoor domestic burning for cooking and heating homes/buildings. Crop residues and firewood are important sources in some parts of China, especially in areas with higher predicted background concentrations in this study and – whilst this can be an important source of indoor air pollution and associated human health concerns – here we focus on the potential contributions to ambient air. The following assumptions were made:

1. A fraction of traditional and improved combustion stoves was also calculated by assuming improved technologies are introduced as described by Bond et al. The percentage of improved stoves was assumed to increase from 34% to 84% for indoor crop residue burning and from 37% to 85% for indoor firewood burning (see Table 1). 2. EFs were assumed stable over time for the individual technology as shown in Table 1 and the average values reported in Shen et al.’s research was adopted; 3. BaP EFs were assumed to be reduced by 40% when improved stoves are used for indoor crop residue burning and indoor firewood burning (Table 1). At the same time, half the indoor crop residue and indoor firewood burning activities were assumed to be reduced due to urbanization or other alternatives (e.g. induction cookers) introduced to rural residents for cooking and heating. It has been projected that half of the rural areas in 2007 could become urbanized before 2030, which is based on the urbanization rate of China in the past 10 years (1% each year conservatively) as reported by World Bank, and an assumption that this rate is maintained until 2030 in regions described in 4 below. Indoor biomass burning is banned in urban areas in China; 4. The technology improvement and biomass burning reduction by urbanization or the other alternatives were performed in the regions of China where the indoor biomass (crop residue and firewood) burning was > 50% to all sources or in the regions with air backgrounds > 1 ng/m³. 5. Open fire burning of agricultural waste is prohibited or regulated in many countries or regions. China also has released a draft version of the ‘Law of People’s Republic
China on the Prevention and Control of Air Pollution’ in which open burning of biomass in densely inhabited districts, areas near airports or the main traffic ways should be forbidden. All open fire agricultural waste burning was assumed to be successfully banned by 2030.

Table 1. Percent usage of different technologies in each sector (EFs mg/tonnes*10)

<table>
<thead>
<tr>
<th>Coal (Sc1) Sectors</th>
<th>Energy production</th>
<th>Industry</th>
</tr>
</thead>
<tbody>
<tr>
<td>No control</td>
<td>Control</td>
<td>No control</td>
</tr>
<tr>
<td>2007</td>
<td>30% (1.2)</td>
<td>70% (1.4×10^2)</td>
</tr>
<tr>
<td>2030</td>
<td>1.8% (1.2)</td>
<td>98.2% (1.4×10^2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Biomass (Sc2) Activities Technology</th>
<th>No control</th>
<th>Control</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indoor crop residue burning Traditional stove</td>
<td>66% (1.8)</td>
<td>34% (0.69)</td>
</tr>
<tr>
<td>Improved stove</td>
<td>63% (1.5)</td>
<td>37% (0.56)</td>
</tr>
<tr>
<td>Indoor firewood burning Traditional woodstove</td>
<td>16% (1.8)</td>
<td>84% (0.69)</td>
</tr>
<tr>
<td>Improved woodstove</td>
<td>15% (1.5)</td>
<td>85% (0.56)</td>
</tr>
</tbody>
</table>

*Notes: the unit of EFs, mg/tonnes, means the amount of BaP (mg) released by burning one tonne of coal or biomass

**Outcomes predicted by the future scenarios**

By adopting improved technology and EFs in Sc1, BaP emissions would decline by 90% and 75% by 2030 in the energy production and industry sectors, respectively, from coal consumption in selected regions in Sc1. The total annual emission would decrease to ca. 900 tonnes/yr in mainland China. By adopting improved stoves and EFs and the assumed urbanization scenario in Sc2, BaP emission would decline by 70% from indoor crop residue and firewood burning by 2030 in selected regions in Sc2. The total annual emission would decrease to ca. 610 tonnes/yr in mainland China. Since the two scenarios don’t conflict, if implementing Sc1+Sc2, the total annual emission would decrease to ca. 470 tonnes/yr in mainland China.

Figure 5-6 show how more efficient Sc2 is than Sc1 in reducing the regional levels of BaP in air and freshwater. The areas where regional background concentrations would exceed 2.5 ng/m^3 and 1 ng/m^3 in air are reduced by ca. 19% and 6% respectively in Sc1 and ca. 51% and 40% in Sc2. Technology improvement for coal consumption is efficient in reducing backgrounds to < 2.5 ng/m^3 only in areas such as Shanxi and boundary of north Ningxia and Inner Mongolia where there are coal mines (Figure 6). Implementation of the biomass burning and consumption control in Sc2 would reduce the regional concentration to < 2.5 ng/m^3 in the northeast provinces, NCP, Jiangsu, Anhui, Sichuan and Guangxi. Indeed, it would reduce BaP levels in large areas in these regions below the 1 ng/m^3 annual guideline value.
For freshwater (Figure S9), the areas where regional backgrounds would exceed 2.8 ng/L are reduced by ca. 20% in Sc2 but show almost no reduction in Sc1, and those that would exceed 15 ng/L are reduced by ca. 20% and 50% respectively in Sc1 and Sc2. Technology improvement on coal consumption in Sc1 would have little effect in reducing freshwater backgrounds to < 2.8 ng/L but would work in small regions in north Ningxia, Gansu and Yunnan in reducing the background concentration to <15 ng/L. Implementation of Sc2 would be efficient in reducing the background level to < 15 ng/L in northeast China, east Sichuan, south Henan and Hubei, and it is efficient in southeast China in reducing backgrounds to < 2.8 ng/L.

The current commitments in government regulations and action plans for air pollution prevention and control focus mainly on reducing coal usage or improving technology on coal consumption. These scenarios suggest that if greater efforts were put into biomass burning control and technology improvement at the same time, as shown in Figure 5-6 (Sc1+2), the areas with air background exceedance of 2.5 ng/m³ and 1 ng/m³ could be reduced by 82% and 54% respectively; and for freshwater backgrounds exceedance of 2.8 ng/L and 15 ng/L, it could be reduced by 34% and 65%. It is also necessary to reduce emissions to both the regional grid cell and to its surrounding area for effective pollution control considering the emission and input from surrounding areas will also influence regional contamination (Figure S10).

This section provides an illustration of the model application in the future scenario discussions above. SESAMe v3.0 can perform well on assessing the efficiency of potential implements made by governments or scientific research on preventing or controlling pollution nationally or regionally. We stress that the scenarios are hypothetical and make no claim about their likely development in the future.

Potential future applications for SESAMe v3.0 as a pollution management tool

In reality, future Chinese emission scenarios will be determined by a complex combination of driving forces such as socio-economic development, large scale state intervention, technology development, climate change and so on. They are evolving dynamically with high uncertainty, so no realistic future scenarios can be predicted confidently. However, research into possible future scenarios can provide useful information to support decision/policy makers to prepare for the challenge of reducing environmental pollution in the future.

It has been demonstrated in this study that utilizing models such as SESAMe v3.0 for both current and future scenario evaluation could provide valuable information for decision-making on emission reduction strategies and future pollution management. Assessment of
current multi-media BaP concentrations across China assists in the identification of which regions would be most affected by the implementation of the two considered scenarios. Major emission sources were also considered when selecting regions for study. It can, therefore, be considered an economical way to evaluate the potential of commitments for pollution control in selected regions rather than in the whole country. Multi-media models have been selected for risk evaluation or pollution management and decision-making by a wide range of researchers and government institutions\textsuperscript{68-71}. SESAME v3.0, as a multi-media model, has the advantage of supporting science and decision-making for the evaluation of future pollution reduction and management.

Figure 5. Cumulative frequency of BaP concentration in air (left) and in freshwater (right)

Figure 6. BaP air concentration in 2007, Sc1, Sc2 and Sc1+Sc2

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Supporting information

Additional information on description of methods, input model parameters, the literature for collecting measured data and the output figures can be found in supporting information document. This information is available free of charge via the Internet at http://pubs.acs.org.

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