Modeling BVOC isoprene emissions based on a GIS and remote sensing database

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This paper presents a geographic information systems (GIS) model to relate biogenic volatile organic compounds (BVOCs) isoprene emissions to ecosystem type, as well as environmental drivers such as light intensity, temperature, landscape factor and foliar density. Data and techniques have recently become available which can permit new improved estimates of isoprene emissions over Hong Kong. The techniques are based on Guenther et al.’s (1993, 1999) model. The spatially detailed mapping of isoprene emissions over Hong Kong at a resolution of 100 m and a database has been constructed for retrieval of the isoprene maps from February 2007 to January 2008. This approach assigns emission rates directly to ecosystem types not to individual species, since unlike in temperate regions where one or two single species may dominate over large regions, Hong Kong’s vegetation is extremely diverse with up to 300 different species in 1 ha. Field measurements of emissions by canister sampling obtained a range of ambient emissions according to different climatic conditions for Hong Kong’s main ecosystem types in both urban and rural areas, and these were used for model validation. Results show the model-derived isoprene flux to have high to moderate correlations with field observations (i.e. $r^2 = 0.77$, $r^2 = 0.63$, $r^2 = 0.37$) for all 24 field measurements, subset for summer, and winter data, respectively) which indicate the robustness of the approach when applied to tropical forests at detailed level, as well as the promising role of remote sensing in isoprene mapping. The GIS model and raster database provide a simple and low cost estimation of the BVOC isoprene in Hong Kong at detailed level. City planners and environmental authorities may use the derived models for estimating isoprene transportation, and its interaction with anthropogenic pollutants in urban areas.

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1. Introduction

Biogenic volatile organic compounds (BVOCs) emitted from vegetation have significant impacts at global scale, on tropospheric chemistry, carbon budget, ozone formation, and contribute to global climate change. BVOCs are more reactive than any anthropogenic volatile organic compounds (VOCs) on a global scale and they are the key elements in the formation of ozone. Ozone is formed by interaction of nitrogen oxides (NOx), volatile organic compounds (VOCs), and sunlight, where NOx and VOC are from anthropogenic sources such as combustion of vehicles, power plants, and natural sources such as forest. Lamb et al. (1987) found that forests are the major source (almost 90%) of BVOC, with the rest from agricultural and scrub lands. Studies of BVOC have been conducted in the last two decades and many have attempted to parameterize the environmental factors influencing BVOC emission from plants (Guenther et al., 1993, 1999; Wang et al., 2003; Chen et al., 2009; Tsui et al., 2009). Large uncertainties are found in the models due to great variability of emissions according to different parameters, e.g. plant species, biomass, climatic factors, as well as differences in validation approaches (Tsui et al., 2009). These uncertainties are particularly significant in tropical regions since the emission rates of most tropical plant species are not known and are not reported in global emission databases. Two studies in Hong Kong (Tsui et al., 2009; Leung et al., 2010) have carried out laboratory measurements of emission rates for a few selected woody forest species, but measured rates were observed to be lower than those in the literature for the same species, possibly due to the difference between laboratory and field environments.
Additionally, the wide variability in rates between tropical forest species (Guenther et al., 1995) suggest that multiplying up from species to landscape level, as is normally done for modeling, would give significant error. In Hong Kong, the vegetation is extremely diverse with up to 300 different species in one hectare (Dudgen and Corlett, 2004). It is then a challenging task to accurately model and map BVOC emissions in Hong Kong at a spatially detailed level.

BVOC emissions are usually parameterized by a set of factors such as standard emission rates for particular vegetation types, levels of foliar density, light and temperature factors. The standard emission rates have generally been assigned based on previous studies which measured BVOC emissions over vegetation canopies in major world ecosystems. However, although the tropics contribute over 80% of global isoprene emissions (Guenther et al., 2006) and isoprene comprises 44% of all BVOC emissions (Guenther et al., 1995), few estimates are from tropical regions. Geron et al. (1994) modeled isoprene emission rates for the eastern United States and found levels 5–10 times higher than for models developed in other countries. This suggests low transferability. Thus accurate estimates of BVOC emissions from tropical landscapes are needed.

Remote sensing techniques and high-resolution data are now available which can be integrated into a BVOC emission model for estimating isoprene emissions over Hong Kong. Isoprene emission rates \((E)\) can be calculated using Eq. (1) (Guenther et al., 1993, 1999):

\[
E \text{ (mgC} \, \text{m}^{-2} \text{h}^{-1}) = \varepsilon D \gamma_T \gamma_P, \tag{1}
\]

where \(\varepsilon\) is the isoprene emission capacity for a landscape (\(\mu\text{gC} \,(\text{leaf dry weight})^{-1} \, \text{h}^{-1}\)); \(D\) is the foliar density (leaf dry matter \(\text{m}^{-2}\) of ground); \(\gamma_T\) is the coefficient representing the influence of temperature on emissions, and \(\gamma_P\) is the coefficient representing the influence of light intensity on emissions.

This standard equation is controlled by standard conditions, e.g. leaf temperature of 30°C and photosynthetically active radiation (PAR) of 1000 \(\mu\text{mol} \, \text{m}^{-2} \, \text{s}^{-1}\). Geron et al. (2000) found that most isoprene is emitted under standard conditions, but adjustments are needed for variable temperature and light conditions in this study. For validation of the model estimates, 24 samples of ambient isoprene concentrations collected from different ecosystem types on 10 days during summer and winter in 2007 were available.

The objective of this study is to devise a GIS model for obtaining isoprene concentrations over Hong Kong at high spatial and temporal resolution. This model uses the basic isoprene emission model of ecosystem types by Guenther et al. (1995), and spatially detailed maps of temperature, foliar density and photosynthetically active radiation obtained by fieldwork and observations combined with satellite images.

### 2. Methodology

Eq. (1) shows the method for computing the isoprene emission rates \((E)\) with different input parameters. These parameters including temperature \((\gamma_T)\), foliar density \((D)\), and PAR \((\gamma_P)\) which were based on satellite image data resampled to a 100 m grid size. Since
the field work for collecting ambient isoprene concentration was carried out in 2007, the temperature and PAR data from February 2007 to January 2008 were acquired from the Hong Kong Observatory. These data were collected on an hourly basis, and only daytime hours were selected. In Hong Kong, the year 2007 was the fifth warmest year since 1884 (HKO, 2012). The annual mean temperature of 23.7 °C was 0.7 °C higher than normal. The year 2007 was also drier than usual. The annual rainfall of 1706.9 mm was about 23% below normal (HKO, 2012). The overall method (Fig. 1) will be elaborated in the following sections.

2.1. Isoprene emission capacity (ε)

In response to a need for accurate distribution maps of vegetation types, a land use/land cover map at 10 m resolution was used. Nine classes of land use/land cover namely: industrial, residential, agricultural, mixed forest, grassland, water, shrubland, shrubby grassland and others were identified. The isoprene emission capacities (ε) from Guenther et al.’s (1995) global database and Tsui et al.’s (2009) local data were assigned to five vegetative classes (listed in Table 1).

Table 1

<table>
<thead>
<tr>
<th>Class</th>
<th>Isoprene emission capacity, ( \varepsilon ) (μg C g(^{-1}) h(^{-1}))</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agricultural</td>
<td>5</td>
<td>Guenther et al. (1995)</td>
</tr>
<tr>
<td>Mixed forest</td>
<td>18.14</td>
<td>Tsui et al. (2009)</td>
</tr>
<tr>
<td>Grassland</td>
<td>24</td>
<td>Guenther et al. (1995)</td>
</tr>
<tr>
<td>Shrubland</td>
<td>16</td>
<td>Guenther et al. (1995)</td>
</tr>
<tr>
<td>Shrubby grassland</td>
<td>24</td>
<td>Guenther et al. (1995)</td>
</tr>
</tbody>
</table>

A program was written in ESRI® ArcGIS™ 9.2 software to calculate the hourly isoprene emission rates (Ε) with inputs of other parameters using Eq. (1). This program first creates a set of mesh polygons (e.g. grid cell of 100 m × 100 m, which is the resolution of the study). Then the land cover/land use data is projected to the same plane and intersected with the mesh polygons. The resulting polygons at 100 m resolution contain information of different land type and then can be used to calculate the isoprene emission capacities (ε) from Table 1. Fig. 2 shows the workflow of this program and Fig. 3 shows the isoprene emission capacity over Hong Kong. Similar techniques were applied to other input parameters such as foliar density, PAR and temperature factors. Finally, these four parameters were input to Equation 1 to generate maps of isoprene emission rates over Hong Kong on an hourly basis.

2.2. Foliar density (D)

In this study, a site-specific allometric model for foliar density (D) (leaf dry matter in g m\(^{-2}\)) was established by harvesting 75 trees, based on the relationship between Diameter at Breast Height (DBH), and leaf dry matter (Nichol and Sarker, 2011). The Ratio Vegetation Index (RVI) was calculated dividing the NIR wavelength by the red wavelength from a geometrically, radiometrically, and atmospherically corrected SPOT 5 image acquired on 31 December, 2006. The RVI probably is the first vegetation index to derive Leaf Area Index (LAI). Jordan (1969) used a ratio between two wavelengths at 800 nm and 675 nm to derive LAI. In this study, the RVI image was regressed against the leaf dry matter measured in 20 forest plots of 30 m diameter, and a strong correlation was observed between image derived RVI and leaf dry matter \( r^2 = 0.81 \) (Fig. 4a). This relationship (leaf dry matter = 3.33 × RVI + 6.57) was used to generate the foliar density map (Fig. 4b). In Hong Kong’s sub-tropical evergreen forests, few deciduous and non-tropical species occur, thus it is assumed that foliar density will not vary significantly by season.

2.3. Photosynthetically active radiation factor (\( \gamma_P \))

A key factor in isoprene emission is the amount of light incident (PAR) receiving on the leaf surface. This can be determined by the parameter leaf area index. Eq. (2) summarizes the relationship between PAR factor (\( \gamma_P \)), PAR flux and LAI (Guenther et al., 1993, 1999):

\[
\gamma_P = \frac{\alpha CIQ}{(1 + \alpha^2 Q^2)^{1/2}}
\]

where \( Q \) is the flux of PAR (μmol m\(^{-2}\) s\(^{-1}\)), \( \alpha = 0.001 + 0.00085 \) LAI, \( C_I = 1.42 \) exp\(-0.3 \) LAI.

In this study, the PAR flux (Q) was calculated based on the hourly solar radiation observed by the Hong Kong Observatory. The solar radiation MJ m\(^{-2}\) was transferred to PAR (μmol m\(^{-2}\) s\(^{-1}\)) for incident light reaching the earth surface over the period where MJ m\(^{-2}\) = (0.5 x 1,000,000)/(0.21 x 3600) μmol m\(^{-2}\) s\(^{-1}\). The maximum and minimum of PAR are <100 and >2500 (μmol m\(^{-2}\) s\(^{-1}\)) observed in cloudy winter and sunny summer time, respectively. In addition, LAI was measured in 11 forest plots of 30 m diameter using a LAI-2000 Plant Canopy Analyzer and the LAI data were regressed against the RVI image. A high correlation \( r^2 = 0.69 \) was observed between field LAI and the RVI image (Fig. 5a). Fig. 5b shows the LAI image derived from the RVI index. Fig. 5c and d shows the derived PAR (\( \gamma_P \)) on July 10, 2007, 3 p.m. local time and January 18, 2008, 3 p.m. local time where the PAR fluxes are ca. 2003 and ca. 1322 μmol m\(^{-2}\) s\(^{-1}\), respectively. Since the urban areas have no LAI values observed on the RVI image, the PAR values of urban areas appear zero (Fig. 5c and d).
2.4. Temperature factor ($\gamma_T$)

Geron et al. (2000) and Guenther et al. (2003) reported that temperature is the most important variable in isoprene emission estimation, and the temperature factor can be calculated using Eq. (3) (Guenther et al., 1993, 1999):

$$\gamma_T = \frac{E_{opt} C_{T2} \exp(C_{T1} x)}{C_{T2} - C_{T1} (1 - \exp(C_{T2} x))}$$

(3)

where $E_{opt}$ is the maximum normalized emission capacity (=1.9), $C_{T1}$ and $C_{T2}$ are the empirical coefficients for energy of activation and deactivation (=95 and =230, respectively), $x = (1/T_{opt} - 1/T)/R$, $T$ is the current leaf surface temperature (in K), $T_{opt}$ is the constant temperature (=312.5 K), and $R$ is the gas constant (=0.00831).

In this study, the current leaf surface temperature ($T$) was generated from 18 ground stations from the Hong Kong Observatory. The 18 temperature stations were then interpolated over the study area using the IDW method. The hourly temperature images were output from the model. Fig. 6a and b shows the temperature factors ($\gamma_T$) calculated using Eq. (3) on July 10, 2007, 3 p.m. local time and January 18, 2008, 3 p.m. local time, respectively.

Finally, the isoprene fluxes (mg C g$^{-1}$ h$^{-1}$) for Hong Kong were calculated for every hour over the period. Fig. 7 shows examples of isoprene fluxes, on July 10, 2007, 3 p.m. local time, January 18, 2008, 3 p.m. local time, and the annual isoprene fluxes, respectively.

2.5. Validation

A total of 24 air samples on 10 days were obtained in the field during 2007. Measurements were taken from different vegetation structural types such as forest, shrubland and grassland within Hong Kong’s country parks. Air was captured in vacuum canisters and GPS were used for locating the field positions for relation to the satellite images. These canisters were transported to the Hong Kong Polytechnic University for chemical analysis by gas chromatography. More details are given in Chen et al. (2009).

Comparisons between field ambient concentrations and modeled emission outputs were made for all 24 data samples from grassland, shrubland and forest (Fig. 8a), which were subset for summer (Fig. 8b) and winter data (Fig. 8c). Results suggest that the model-derived isoprene flux had moderate to high correlations with field observations (i.e., $r^2 = 0.77$, $r^2 = 0.63$, $r^2 = 0.37$ for all 24 field measurements, for whole year, summer, and winter data, respectively) which indicates the robustness of the approach when applied to tropical forests at detailed level, as well as the promising role of remote sensing in isoprene mapping.

2.6. Estimates of yearly emission

Hourly isoprene emissions covering Hong Kong have been modeled in this study. High-resolution isoprene maps with high spatial detail can be used for emission control at both local district and city levels. Yearly isoprene emission can also be calculated using 5475 images in the form of a raster database. Since the isoprene maps do not cover the entire Hong Kong territories, an average value based on total isoprene emissions for areas of vegetative types was estimated. Table 2 compares total isoprene emissions and isoprene emissions per area between Hong Kong, Beijing and globally. The yearly isoprene emission for Hong Kong estimated in this study ($6.8 \times 10^6$ g C year$^{-1}$) is lower than that of Tsui et al. (2009) ($2.6 \times 10^6$ g C year$^{-1}$) and Leung et al. (2009) ($7.1 \times 10^6$ g C year$^{-1}$). Yearly isoprene emission per land area in this study ($1.9 \times 10^6$ g C km$^{-2}$ year$^{-1}$) is also lower than that of Tsui et al. (2009) ($7.8 \times 10^6$ g C km$^{-2}$ year$^{-1}$). These disagreements may come from (i) different years of data: we used temperature and
Fig. 4. (a) Comparison between leaf dry weight and ratio vegetation index (RVI) SPOT image, from 20 forest plots and (b) foliar density image.
Fig. 5. (a) Comparison between LAI field data and LAI image derived from RVI index, (b) LAI image, PAR factor (γ) images on (c) July 10, 2007, 3 p.m. local time and (d) January 18, 2008, 3 p.m. local time.
Fig. 5. (Continued).
Fig. 6. Temperature factor ($\gamma_T$) derived from hourly temperature data from HKO, images on (a) July 10, 2007, 3 p.m. local time and (b) January 18, 2008, 3 p.m. local time.
Fig. 7. Isoprene emission rate (100 m resolution) on (a) July 10, 2007, 3 p.m. local time, (b) January 18, 2008, 3 p.m. local time and (c) annual basis.
PAR data from February 2007 to January 2008, whereas Tsui et al. (2009) made use of data from August 2004 to July 2005 and Leung et al. (2009) calculated isoprene emission in 2006; (ii) different types of input data: our study used hourly temperature and hourly PAR data over the period whereas Tsui et al. (2009) used monthly averaged temperature and PAR data; (iii) different estimates of isoprene capacities: in this study, isoprene capacities from both Tsui et al. (2009) and Guenther et al. (1995) were adopted; and (iv) different study areas, since our study area does not entirely cover Hong Kong.

However, Tsui et al.’s (2009) measured species represented only 76% of Hong Kong’s total estimated BVOC and Guenther et al. (1995) used a global database, which does not include Hong Kong’s dominant species. Leung et al. (2009) also working in Hong Kong used global isoprene emission capacities based on the Model of Emissions of Gases and Aerosols from Nature (MEGAN) (Guenther et al., 2006) whereas the emission rates of Hong Kong temperate secondary forests are not known and the emissions for the dominant tree species are not reported in global emission databases. In addition, yearly isoprene emission per area in this study (1.9 × 10⁶ gC km⁻² year⁻¹) is lower than Tsui et al. (2009)’s study (7.8 × 10⁶ gC km⁻² year⁻¹) and global estimation (7.5 × 10⁶ gC km⁻² year⁻¹), but higher than Beijing’s study (8.9 × 10⁵ gC km⁻² year⁻¹), since Hong Kong has a higher percentage of vegetation (80%) and forest covers (18%) than Beijing with only 7% of vegetation cover (Wang et al., 2003). Grassland and forest are the major contributors of isoprene emission among different vegetation types, with 41% and 39% of the total, and grassland also has the highest yearly isoprene emission per area (7.8 × 10⁵ gC km⁻² year⁻¹) (Table 3).

Table 2
Yearly isoprene emissions for different cities/regions.

<table>
<thead>
<tr>
<th>City/region</th>
<th>Yearly isoprene emission (gC year⁻¹)</th>
<th>Yearly isoprene emission per area (gC km⁻² year⁻¹)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hong Kong (February 2007 to January 2008)</td>
<td>6.8 × 10⁸</td>
<td>1.9 × 10⁶</td>
<td>This study</td>
</tr>
<tr>
<td>Hong Kong (summer 2004 to summer 2005)</td>
<td>2.6 × 10⁸</td>
<td>1.9 × 10⁶</td>
<td>Tsui et al. (2009)</td>
</tr>
<tr>
<td>Hong Kong (2006)</td>
<td>7.1 × 10⁸</td>
<td>7.8 × 10⁶</td>
<td>Leung et al. (2009)</td>
</tr>
<tr>
<td>Beijing</td>
<td>7.7 × 10⁹</td>
<td>8.9 × 10⁵</td>
<td>Wang et al. (2003)</td>
</tr>
<tr>
<td>Global</td>
<td>4.8 × 10¹⁴</td>
<td>7.5 × 10⁶</td>
<td>Guenther et al. (1995)</td>
</tr>
</tbody>
</table>

Table 3
Yearly isoprene emissions for different vegetation types within Hong Kong.

<table>
<thead>
<tr>
<th>Vegetation class</th>
<th>Yearly isoprene emission (gC year⁻¹)</th>
<th>Yearly isoprene emission per area (gC km⁻² year⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agriculture</td>
<td>5.5 × 10⁴</td>
<td>7.9 × 10³</td>
</tr>
<tr>
<td>Forest</td>
<td>5.2 × 10⁴</td>
<td>7.4 × 10³</td>
</tr>
<tr>
<td>Shrubland</td>
<td>2.5 × 10⁵</td>
<td>3.6 × 10³</td>
</tr>
<tr>
<td>Grassland</td>
<td>5.5 × 10⁵</td>
<td>7.8 × 10³</td>
</tr>
</tbody>
</table>
3. Discussion and conclusion

This study has demonstrated a GIS model to relate isoprene emissions to ecosystem type using remote sensing technology to obtain isoprene concentrations at high spatial detail over Hong Kong. The derived estimates are likely to be more accurate than other studies (Tsui et al., 2009; Leung et al., 2009), because hourly temperature and PAR data were used as inputs, to produce a whole year hourly isoprene database (a total of 5475 images). This study also validated the model outputs using field ambient concentrations at precise locations and precise times. Results show that the model-derived isoprene flux has moderate to high correlations with field observations (i.e. $r^2 = 0.77$, $r^2 = 0.63$, $r^2 = 0.37$ for all 24 field measurements in whole year and subset for summer, and winter respectively) which indicates the robustness of the approach when applied to tropical forests at detailed level, as well as the promising role of remote sensing in isoprene mapping. Other BVOCs such as beta-Pinene and Limonene will be mapped in a future study.

While uncertainties in BVOC models may exist based on variations in foliar density, LAI and other environmental stresses, in this study, the foliar density and LAI were measured in the field and averaged from 11 and 20 forest plots of 30 m diameter respectively. The foliar density computed in this study (200–800 g m$^{-2}$) appears similar to other values of primary tropical rainforest (600–1100 g m$^{-2}$) from Alexandre (1981), and temperate deciduous and coniferous forest (375 g m$^{-2}$, 700–1500 g m$^{-2}$, respectively). Most LAI values used in this study are between 3 and 5 which appears lower than Tsui et al. (2009)'s values of 3–7 for Hong Kong, probably because the latter assumed a 100% canopy cover. More field measurements of seasonal foliar density and LAI (fraction of foliar/biomass density over different seasons) will be considered in a future study.

Temperature and PAR are other driving forces of temporal isoprene emission estimates. This study adopted temperature data from 18 ground climate stations and interpolated to the entire area using the IDW method. Although 18 ground stations provide high temporal (hourly) data, their discrete spatial distributions (most are located in urban and suburban areas) do not provide good representation for the entire Hong Kong territories (1100 km$^2$). Integration of the MM5 model with localized climate stations to derive more accurate temperature data would provide a better solution. In addition, PAR data derived from this study is based on a single climatic station. They only represent the PAR values at the climatic station and its immediate neighborhood whereas an assumption of homogenous PAR values over the entire territories is made in this study. More studies by correlating PAR with MODIS cloud products (Platnick et al., 2003) and cirrus cloud observations from Lidar will help to generate more comprehensive PAR maps.

The GIS model and raster database offers a simple and low cost estimation of BVOC isoprene concentration over Hong Kong at detailed level. City planners and environmental authorities may use the derived models for estimating its transportation, and interaction with anthropogenic pollutants in urban areas. In addition, accurate and highly detailed BVOC maps produced in this study are necessary for studying secondary aerosols, since BVOC emissions may play an important role in the formation of photochemical smog. In future urban ecosystem planning, new planting of species with low BVOC emission but with large canopy layers should be considered. Isoprene and other BVOC emissions increase significantly with high temperatures, but, trees with large canopy layers can reduce urban temperatures locally by 6–7 °C (Nichol and Wong, 2005). Thus, since trees are potentially both beneficial and harmful, the GIS model and raster database derived from this study may be used to balance the relative benefits of urban woodlands.

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