Comparing BC mixing state from CAMChem to SP2 measurements

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1 SP2 Measurement

The SP2 instrument measures BC particles in the diameter range from approximately 90 to 400 nm, which is unlikely to represent the total ambient number and mass concentrations of BC (Reddington et al., 2013). In order to compare CAMChem model simulated BC with observations, we estimated the mass fraction of modeled BC in the size range (90–400 nm) corresponding to SP2 measurement.

2 Estimating the mean BC core diameter in primary carbon mode and in accumulation mode

A 4-mode version of the modal aerosol model (MAM4) is applied in CAMChem1.2.2. BC is emitted to the primary carbon mode, and then is transferred to the accumulation mode by condensation of H_2SO_4, NH_3 and SOA and by coagulation (Liu et al., 2012). In primary carbon mode, particles consist of externally mixed BC and OC, whereas in accumulation mode, particles consist of internally mixed BC and non-BC material. SP2 measures the mass size distribution of the BC

particle cores over a calibrated volume equivalent diameter (VED) range of 55–400 nm, and the number-detection efficiency at sea level pressure is reported to be one for BC above 90 nm VED (Schwarz et al., 2010a). So following Reddington et al., 2013, we use 90 nm as the lower bound here. Both modes assume lognormal distribution as is shown in table 1. σ_g is fixed but geometric

mean diameter can change according to total mass and total number of aerosol particles in that mode.

The mean BC core diameter in accumulation mode is estimated as:

$$D_{\text{core}} = (D_{\text{mixed}}^3 \times f_{\text{BC}})^{\frac{1}{3}},$$

where D_{core} is the mean diameter of BC core,D_{mixed} is the mean diameter of internally mixed particles (**extracted from model**), and f_{BC} is the volume fraction of BC in accumulation mode.

MAM4	σ_g	10th and 90th percentiles (μm)
Accumulation	1.8	0.058-0.27
Primary Carbon	1.6	0.039-0.13

Table 1: Parameters of Lognormal Distribution.

3 Compute Volume Fraction Corresponding to Lognormal Distribution

The CDF of number distribution in the size range between d_1 and d_2 is:

$$N(d_1, d_2) = \frac{1}{\ln\sigma_\mathrm{g}\sqrt{2\pi}}\int_{d_1}^{d_2} e^{-}\frac{(\ln r - \ln r_g)^2}{2\ln^2\sigma_\mathrm{g}}\mathrm{d}(\ln r),$$

where r_g is mean geometric diameter (extracted from model, varying temporally and spatially). The mean volume is proportional to function of the form:

$$\begin{aligned}N(d_1, d_2) &= \frac{1}{\ln\sigma_\mathrm{g}\sqrt{2\pi}}\int_{d_1}^{d_2} r^3 e^{-}\frac{(\ln r - \ln r_g)^2}{2\ln^2\sigma_\mathrm{g}}\mathrm{d}(\ln r)\\ &= \frac{e^{\frac{k^2}{2}\ln^2\sigma_g + k\ln r_g}}{\ln\sigma_\mathrm{g}\sqrt{2\pi}}\int_{d_1}^{d_2} r^3 e^{-}\frac{(\ln r - \ln r_\mathrm{gv})^2}{2\ln^2\sigma_\mathrm{g}}\mathrm{d}(\ln r),\end{aligned}$$

where the volume mean diameter is of the form $\mathrm{lnr_{gv}} = \mathrm{lnr_g} + 3\ln\sigma_\mathrm{g}$.
So BC mass fraction (in the size range between 90–400 nm) in a mode (Figure 1) is derived by:

$$\begin{aligned}F(\mathrm{d_1}, \mathrm{d_2}) &= \frac{\frac{1}{\ln\sigma_\mathrm{g}\sqrt{2\pi}}\int_{d_1}^{d_2} r^3 e^{-\frac{(\ln r - \ln r_g)^2}{2\ln^2\sigma_\mathrm{g}}}\mathrm{d}(\ln r)}{\frac{1}{\ln\sigma_\mathrm{g}\sqrt{2\pi}}\int_{0}^{+\infty} r^3 e^{-\frac{(\ln r - \ln r_g)^2}{2\ln^2\sigma_\mathrm{g}}}\mathrm{d}(\ln r)}\\ &= \frac{\frac{e^{\frac{k^2}{2}ln^2\sigma_g + k\ln r_g}}{\ln\sigma_\mathrm{g}\sqrt{2\pi}}\int_{d_1}^{d_2} e^{-\frac{(\ln r - \ln r_\mathrm{gv})^2}{2\ln^2\sigma_\mathrm{g}}}\mathrm{d}(\ln r)}{\frac{e^{\frac{k^2}{2}ln^2\sigma_g + k\ln r_g}}{\ln\sigma_\mathrm{g}\sqrt{2\pi}}\int_{0}^{+\infty} e^{-\frac{(\ln r - \ln r_\mathrm{gv})^2}{2\ln^2\sigma_\mathrm{g}}}\mathrm{d}(\ln r)}\\ &= \frac{1}{\ln\sigma_\mathrm{g}\sqrt{2\pi}}\int_{d_1}^{d_2} e^{-}\frac{(\ln r - \ln r_\mathrm{gv})^2}{2\ln^2\sigma_\mathrm{g}}\mathrm{d}(\ln r)\\ &= \frac{1}{2}[\mathrm{erf}(\frac{\ln d_2 - \ln r_\mathrm{gv}}{\sqrt{2}\ln\sigma}) - \mathrm{erf}(\frac{\ln d_1 - \ln r_\mathrm{gv}}{\sqrt{2}\ln\sigma})],\end{aligned}$$

Within the size range (90–400 nm), the ratio of BC mass in each mode to total BC mass is computed as:

$$\begin{aligned}f_\mathrm{accu} &= \frac{F_\mathrm{accu}(d_1, d_2)M_\mathrm{accu}}{F_\mathrm{accu}(\mathrm{d}_1, d_2)M_\mathrm{accu} + F_\mathrm{pc}(d_1, d_2)M_\mathrm{pc}}\\ f_\mathrm{pc} &= \frac{F_\mathrm{pc}(d_1, d_2)M_\mathrm{pc}}{F_\mathrm{accu}(d_1, d_2)M_\mathrm{accu} + F_\mathrm{pc}(d_1, d_2)M_\mathrm{pc}}\end{aligned}$$

$$f_\mathrm{accu} + f_\mathrm{pc} = 1,$$

where f_accu is the fraction of BC mass in accumulation mode, f_pc is the fraction of BC mass in primary carbon mode (Figure 2), M_accu and M_pc are BC mass in accumulation mode and primary carbon mode respectively.
In figure 2,
Figure 3 shows monthly BC mass concentration for March.

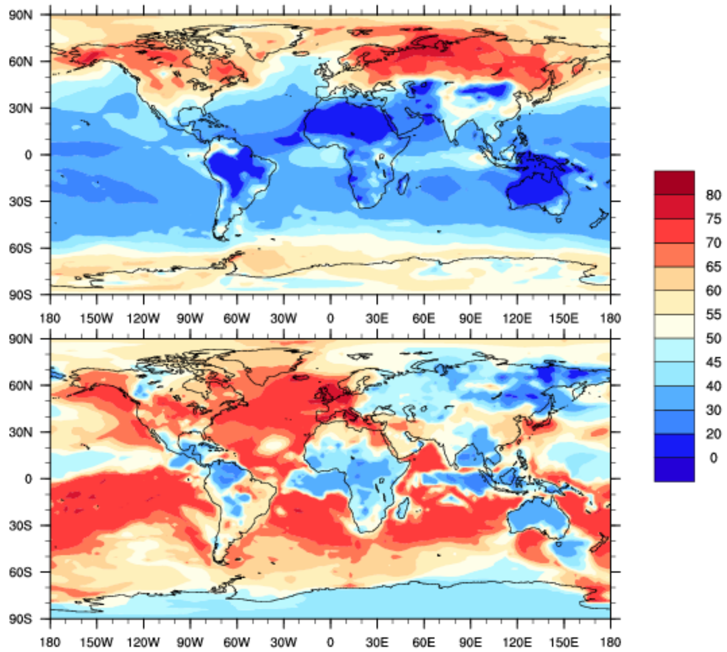

Figure 1: BC mass fraction (%) (between 90 and 400 nm) in primary carbon mode (top) and in accumulation mode (bottom), for surface layer, March.

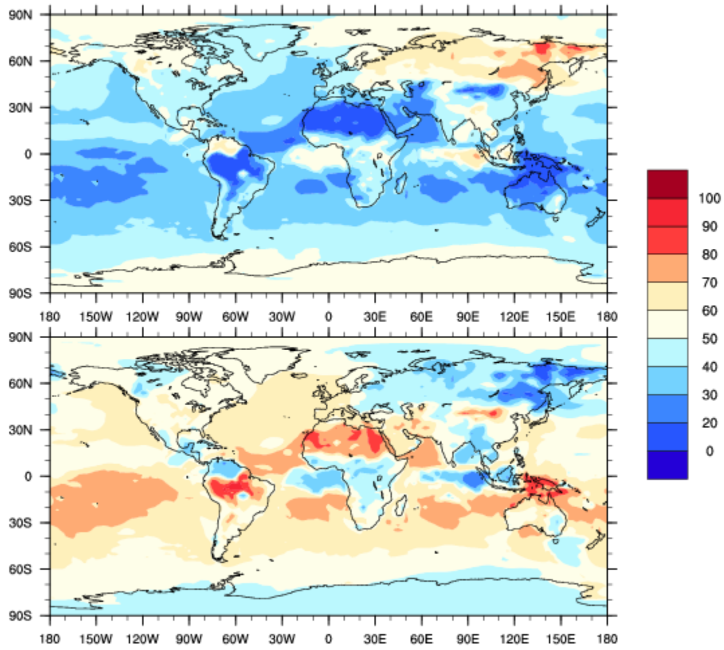

Figure 2: Ratio of BC mass (%) within SP2 size range to total BC mass within SP2 size range, in primary carbon mode (top) and accumulation mode (bottom), for surface layer, March.

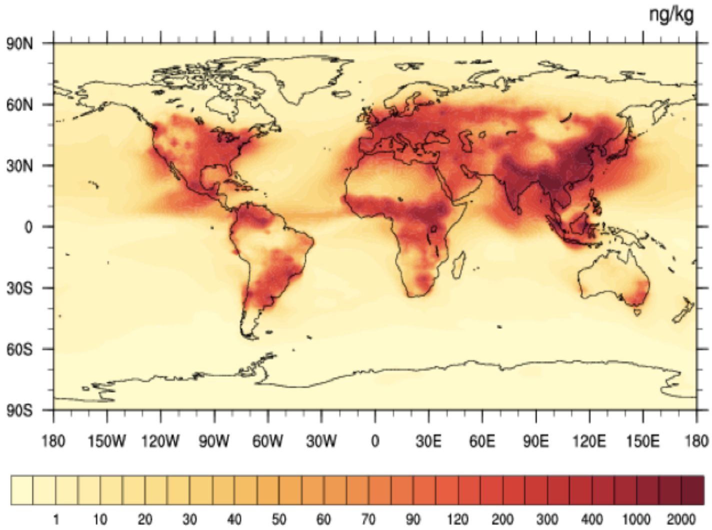

Figure 3: BC mass concentration, for surface layer, March.

References.

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