Supplemental Information for:

Simulating the degree of oxidation in atmospheric organic particles

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Derivation of equations used to treat POA oxidation in CMAQ

Dividing Equation (2) by OC (or the equivalent $12 \times n_{OC}$) and combining with Equation (3), yields a relationship between OM/OC and $\frac{n_O}{n_C}$ or $\frac{n_H}{n_C}$.

$$\frac{n_O}{n_C} = \frac{12}{15} \times \frac{OM}{OC} - \frac{14}{15}$$ Equation (S1)

$$\frac{n_H}{n_C} = \frac{44}{15} - \frac{12}{15} \times \frac{OM}{OC}$$ Equation (S2)

Dividing Equation (S2) by Equation (S1) yields a relationship between $\frac{n_H}{n_O}$ and OM/OC,

$$\frac{n_H}{n_O} = \frac{\frac{44}{12} - \frac{OM}{OC}}{\frac{OM}{OC} - \frac{14}{12}}$$ Equation (4b)

which can be used in an NCOM mass balance to determine moles of oxygen.

$$NCOM = n_H + 16 n_O = n_O \frac{n_H}{n_O} + 16 n_O$$ Equation (S3)

$$n_O = \frac{NCOM}{16 + \frac{n_H}{n_O}}$$ Equation (4a)

Equations (S1) and (S2) allow the determination of $\frac{n_O}{n_C}$ and $\frac{n_H}{n_C}$ without having to explicitly track oxygen and hydrogen species in the model. In addition, these relationships can be used to convert measured OM/OC ratios to $\frac{n_O}{n_C}$ and $\frac{n_H}{n_C}$. Equation (S1) can also be rewritten so that OM/OC is a function of $\frac{n_O}{n_C}$:

$$\frac{OM}{OC} = 1.25 \frac{n_O}{n_C} + 1.167$$ Equation (S4)

Other studies have fit empirical relationships between OM/OC and $\frac{n_O}{n_C}$. Aiken et al.[1] found that data from downtown Mexico City and chamber measurements of SOA and POA fit the equation, $\frac{OM}{OC} = 1.26 \frac{n_O}{n_C} + 1.18$, with an R^2 of 0.997. Sun et al. [2] found that data from Whistler Mountain, British Columbia fit the equation, $\frac{OM}{OC} = 1.33 \frac{n_O}{n_C} + 1.18$, with an R^2 of 0.995. The similarity between these empirical relationships and Equation (S4) support our use of Equation (S4) in Section 3.3 of this paper. Note that the data of Sun et al.[2] were not used by Heald et al.[3] when deriving Equation (2).

Table S1: Measured $\frac{n_O}{n_C}$ and $\frac{n_H}{n_C}$ ratios for OM sources and ambient OM.

OM type	$\frac{n_O}{n_C}$	$\frac{n_H}{n_C}$	Reference
Mobile source POA	0.03-0.05		1, 4
Plastic combustion POA	0.03-0.05		1, 4
Cooking POA	0.1	1.8-1.9	4, 5
Biomass combustion POA	0.3-0.45	1.45-1.8	1, 4, 5
SOA	0.3-0.4	1.5	1, 5
Mexico City fresh urban OM	0.5		1, 6, 7
Aged OM from Mexico City	0.6-0.8		1, 6, 7
Mexico City biomass burning OM	0.3-0.8		6, 7
Mexico City regional OM	0.7		1
Whistler Mountain aged OM	0.9-1.1		2
Whistler Mountain fresher OM	0.6-0.7		2
Pacific NW – younger Asian Layer	0.6		8
Pacific NW – older Asian layer	0.8		8
California central valley	0.5		8

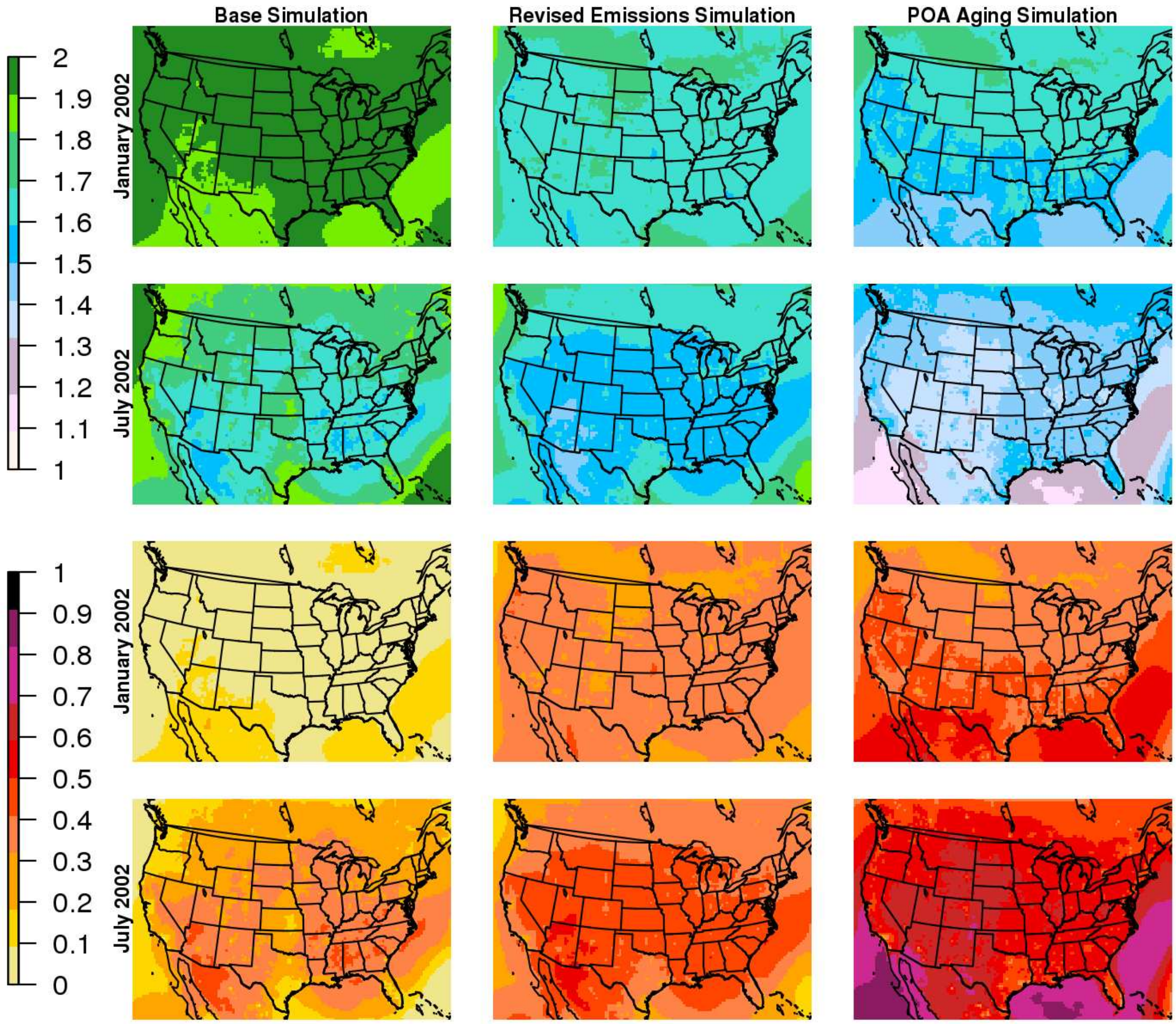

Figure S1. Monthly average $\frac{n_H}{n_C}$ ratios for January 2002 (top), $\frac{n_H}{n_C}$ ratios for July 2002 (2nd from top), $\frac{n_O}{n_C}$ ratios for January 2002 (2nd from bottom), and $\frac{n_O}{n_C}$ ratios for July 2002 (bottom). Results are presented for the basecase simulation (left), the revised emissions simulation (middle) and in the revised emissions + POA aging simulation (right).

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