Box Model for CO_2 in an Urban Atmosphere

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1 Our Box Model

We set up a "box" that has lateral length of Δx and Δy, and height h. From mass-balance of CO_2, we can formulate the time rate of change of CO_2 molar concentration.

$$\Delta x \Delta y h \frac{dC_{bl}}{dt} = Q + u \Delta x h (C_{up} - C_{bl}) + \Delta x \Delta y \frac{dh}{dt}(C_{ent} - C_{bl}) \tag{1}$$

where,

$\mathbf{C}_{bl}$: CO_2 concentration in mol/m^3 for planetary boundary layer.

$\mathbf{C}_{up}$: CO_2 concentration in mol/m^3, for upwind box

$\mathbf{C}_{ent}$: CO_2 concentration in mol/m^3 above boundary layer

Δx **and** Δy: lateral length of the box (m)

Q: emission rate in mol/sec

u: wind speed to the box in m/s

h: boundary layer height in m

Dividing both sides by $\Delta x \Delta y h$ gives

$$\frac{dC_{bl}}{dt} = \frac{q}{h} + \frac{1}{\tau}(C_{up} - C_{bl}) + \frac{1}{h}\frac{dh}{dt}(C_{ent} - C_{bl}) \tag{2}$$

where, τ is the residence time of air over the area of the box ($\tau = \Delta y/u$), and q is the emission rate of CO_2 per unit area (mol m^{-2} s^{-1}) (*see* Seinfeld and Pandis, eq 25.13 and 25.14, p.1098). The first term, second and third terms on the right hand side represent source flux, advection and entrainment, respectively. The entrainment term only applies when boundary layer heigh is increasing ($dh/dt > 0$). One can solve the equation (2) numerically. That is,
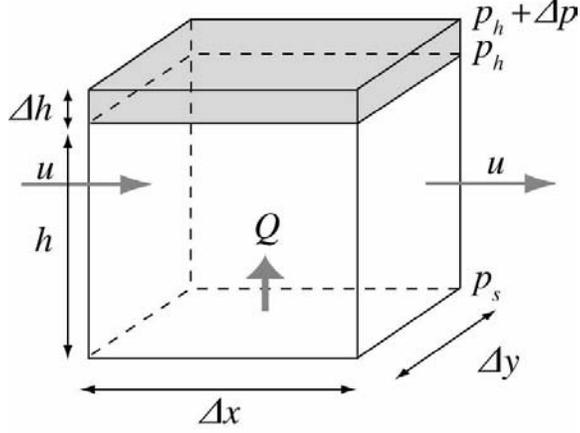
Figure 1: Dimensions and parameters for the box model

$$\frac{C_{bl}^{n+1} - C_{bl}^n}{\Delta t} = \frac{q^n}{h^n} + \frac{1}{\tau}(C_{up}^n - C_{bl}^n) + \frac{1}{h^n}\frac{h^{n+1} - h^n}{\Delta t}(C_{ent}^n - C_{bl}^n) \tag{3}$$

where, $n+1$ and n superscript represent values at time step n and $n+1$, where $t^{n+1} = t^n + \Delta t$

$$C_{bl}^{n+1} = C_{bl}^n + \left[\frac{q^n}{h^n} + \frac{1}{\tau}(C_{up}^n - C_{bl}^n)\right]\Delta t + \frac{h^{n+1} - h^n}{h^n}(C_{ent}^n - C_{bl}^n) \tag{4}$$

Once we know C^n, one can integrate with time to solve C^{n+1}.

2 Concentration and Mixing Ratios

It is important, however, to realize that the air becomes thiner at high altitude. It is convenient to use mixing ratios rather than volume concentrations to express mass-balance equation since mixing ratio is conservative within boundary layer whereas volume concentration of CO_2 change with altitude. From balance of force (Seinfeld and Pandis, p 9),

$$(p(z) - p(z + \Delta z))\Delta A = \rho g \Delta A \Delta z \tag{5}$$

where p is the pressure at altitude z and $z + \Delta z$, ρ, g, are density of air (e.g., kg/m^3) and acceleration due to gravity (m/s^{-2}), pressure is in Pascal. The molar concentration of air at altitude between z and $z + \Delta z$ is:

$$C_{air} = \frac{p(z) - p(z + \Delta z)}{M_{air}g\Delta z} \tag{6}$$

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where, M_{air} is molecular weight of air (28.97 g/mol). Molar concentration of CO_2 is related to the mixing ratio (m_{bl}) of CO_2 as:

$$
\begin{aligned}
C_{bl} &= m_{bl} \cdot C_{air,bl} \\
&= m_{bl} \cdot \frac{(p_s - p_h)}{M_{air}gh}
\end{aligned}
\tag{7}
$$

here, p_s and p_h are the pressure at surface and boundary layer height (h). The source flux and advection terms in equation (2) can be written as (assuming h and p_h does not change with time?):

$$
\frac{dm_{bl}}{dt} = \frac{M_{air}g}{(p_s - p_h)}q + \frac{1}{\tau}(m_{up} - m_{bl})
\tag{8}
$$

For the entrainment term, mass-balance is:

$$
\Delta x \Delta y h C_{bl} = \Delta x \Delta y \Delta h C_{ent} + \Delta x \Delta y (h + \Delta h)(C_{bl} + \Delta C_{bl})
\tag{9}
$$

applying equation (7),

$$
(p_s - p_h)m_{bl} + (\Delta p)m_{ent} = (p_s - p_h + \Delta p)(m_{bl} + \Delta m_{bl})
\tag{10}
$$

Rearrangement and neglecting the second order term $(\Delta p \Delta m_{bl})$ gives:,

$$
\Delta m_{bl} = \frac{\Delta p}{p_s - p_h}(m_{ent} - m_{bl})
\tag{11}
$$

Dividing both sides by Δt, and $\Delta t \to 0$, gives

$$
\frac{dm_{bl}}{dt} = \frac{1}{p_s - p_h}\frac{dp}{dt}(m_{ent} - m_{bl})
\tag{12}
$$

Again, the entrainment term only applies when boundary layer height is increasing (i.e., $dh/dt > 0$ and thus $dp/dt < 0$). Therefore, the full mass-balance equation in terms of mixing ratio and pressure is:

$$
\frac{dm_{bl}}{dt} = \frac{M_{air}g}{(p_s - p_h)}q + \frac{1}{\tau}(m_{up} - m_{bl}) + \frac{1}{p_s - p_h}\frac{dp}{dt}(m_{ent} - m_{bl})
\tag{13}
$$

3   Boundary Layer Height

note: This part will be updated for 2013 meteorological data.

We will use the following harmonic function for the pressure at the top of boundary layer (p_h) as a function of time $(t$ in hours),

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$$p_h(t) = \sum_{k=1}^{m} \left[a_k sin\left(\frac{2\pi kt}{24}\right) + b_k cos\left(\frac{2\pi kt}{24}\right) \right] + a_0 \tag{14}$$

I used up to 4th harmonics (i.e., $m = 4$) to fit PBLH estimated from NAM (North American Mesoscale) model output for Boston from October 18 00 am to October 30 23pm (EST-daylight saving time)

Table 1: Coefficients for harmonic fitting

k	a_k	b_k
1	75.2235	62.8391
2	-29.1925	8.0102
3	-7.4486	6.5066
4	1.9185	-11.6844
$a_0 =$	931.7713	

4   Laboratory Activity

My MATLAB® file is provided for initial model set up. The file has a basic structure to run the model, including the boundary layer height as a function of time. You are encouraged to try sensitivity analysis for various terms. For example,

- set the advection term to zero and adjust the source flux to fit mixing ratio and diurnal amplitude.

- try increasing or decreasing the boundary layer height by x2 or x0.5, see how the model responds.

- change CO_2 in upwind or above, and see model response.

- explore what you think is interesting and reasonable!

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