COMPUTING EXPECTED AEROSOL CONCENTRATIONS
WHEN SOURCE AND DEPOSITION RATES ARE RANDOM

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Computing properties of the distribution of atmospheric aerosol concentrations analytically can be quite difficult for even very simple stochastic models. Baker, et al. (1979) have done work in computing the moments of the concentration under rather restrictive assumptions, one of which is that wet and dry deposition rates are fixed constants. The assumption that the wet deposition rate is constant can be grossly in error, at least in the case of sulfur dioxide, as pointed out by Barrie (1981). This paper shows how to calculate the expected concentration when the deposition rates are fixed within a rainy/dry period, but are allowed to vary between periods.

If transport can be ignored (see Baker, p. 40, for a discussion on when this assumption is reasonable), then concentration at time \( t \), \( c(t) \), will approximately obey

\[
\frac{dc(t)}{dt} = q(t, c(t)) - s(t, c(t)),
\]

where \( q \) and \( s \) are source and sink, respectively.

If the sink is due to deposition, then

\[
s(t, c(t)) = d(t, c(t)) c(t),
\]
where \( d(t, c(t)) \) is the deposition rate. If \( d \) and \( q \) do not depend on \( c \), then we have the following first order linear differential equation:

\[
\frac{dc(t)}{dt} = q(t) - d(t) \cdot c(t).
\]

For a model with fixed source and wet and dry deposition rates, Baker computes moments of \( c \) directly by deriving a pair of partial differential equations involving the density of \( c(t) \). Under less restrictive assumptions, the expected value of \( c \) can be found indirectly by first computing the expected value of \( c \) at times at which rain stops or starts, and then deriving the expected value of \( c \) at an arbitrary time from this information. Let

\[
\begin{align*}
t_0 &= 0 = \text{a time at which precipitation starts}, \\
t_n &= n^{th} \text{ time after } t_o \text{ at which precipitation starts, and} \\
\tilde{t}_n &= \text{time at which } n^{th} \text{ precipitation stops.}
\end{align*}
\]

So, \( 0 = t_0 < \tilde{t}_0 < t_1 < \tilde{t}_1 \ldots \).

Define \( \chi_n = c(t_n) \), and \( \tilde{\chi}_n = c(\tilde{t}_n) \). Then solving equation (1), we obtain:

\[
\chi_{n+1} = \exp\left[-\int_{t_n}^{t_{n+1}} d(t) dt\right] \chi_n \\
+ \exp\left[-\int_{t_n}^{t_{n+1}} d(t) dt\right] \int_{t_n}^{t_{n+1}} q(t) \exp\left[-\int_{t_n}^{t} d(u) du\right] dt \\
= A_n \chi_n + B_n.
\]

Throughout this paper, it will be assumed that \( \{(A_i, B_i)\}_{i=0}^{\infty} \) form an i.i.d. bivariate sequence. From equation (2), we iteratively obtain:
\[ X_n = A_{n-1}(A_{n-2}(\ldots(A_0 X_0 + B_0) \ldots + B_{n-2}) + B_{n-1}) \Rightarrow \]

\[ EX_n = (EA_1)^n EX_0 + EB_1(1 + EA_1 + \ldots + (EA_1)^{n-1}) \Rightarrow \]

\[ (3a) \quad EX_\infty \equiv \lim_{n \to \infty} EX_n = \frac{EB_1}{1-EA_1}, \quad \text{for } EX_0 < \infty. \]

Similarly, define

\[ \bar{A}_n = \exp\left(-\int_{\tilde{t}_n}^{\tilde{t}_{n+1}} d(t)dt\right), \]

\[ \bar{B}_n = \exp\left(-\int_{\tilde{t}_n}^{\tilde{t}_{n+1}} d(t)dt\right) \int_{\tilde{t}_n}^{\tilde{t}_{n+1}} q(t) \exp\left(\int_{\tilde{t}_n}^{t} d(u)du\right) dt, \]

and assume \( \{(\bar{A}_i, \bar{B}_i)\}_{i=0}^\infty \) form an i.i.d. bivariate sequence. Then

\[ (3b) \quad E\bar{X}_\infty \equiv \lim_{n \to \infty} E\bar{X}_n = \frac{EB_1}{1-EA_1}. \]

Now assume that \( d(t) \) and \( q(t) \) are constant during a period of precipitation or dryness, and define

\[ Q^+_n = q(t) \quad \text{for } t \in (\tilde{t}_n, \tilde{t}_n), \]

\[ Q^-_n = q(t) \quad \text{for } t \in (\tilde{t}_n, \tilde{t}_{n+1}), \]

\[ D^+_n = d(t) \quad \text{for } t \in (\tilde{t}_n, \tilde{t}_n), \]

\[ D^-_n = d(t) \quad \text{for } t \in (\tilde{t}_n, \tilde{t}_{n+1}), \]

\[ Y^+_n = \tilde{t}_n - t_n = \text{length of } n'\text{th rainfall}, \]

\[ Y^-_n = t_{n+1} - \tilde{t}_n = \text{length of } n'\text{th dry period}. \]
Then (2) becomes

\[ \begin{align*}
(2') \quad X_{n+1} &= e^{-D_n^+ Y_n^+ - D_n^0 Y_n^0} \\
&\quad \times e^{-D_n^+ Y_n^+} e^{-D_n^0 Y_n^0} \left( 1 - e^{-D_n^+ n} \right) + e^{-D_n^0 Y_n^0} \left( 1 - e^{-D_n^0 n} \right),
\end{align*} \]

for \( D_n^0, D_n^+ > 0 \).

Further, assume that \( \{Q_n^+\}_{n=0}^{\infty}, \{Q_n^0\}_{n=0}^{\infty}, \{D_n^+\}_{n=0}^{\infty}, \{D_n^0\}_{n=0}^{\infty}, \{Y_n^+\}_{n=0}^{\infty}, \{Y_n^0\}_{n=0}^{\infty} \) are all i.i.d. sequences and are mutually independent. Also assume, as in Baker, that the lengths of dry and rainy periods have exponential distributions; i.e., \( P(Y_n^+ > t) = e^{-t/T_+}, \) and \( P(Y_n^+ > t) = e^{-t/T_+}, \) for some constants \( T_+, T_0 \). Then

\[ E e^{-D_n^+ Y_n^+} e^{-D_n^0 Y_n^0} = E \{ e^{-D_n^+ Y_n^+} \} = E \left( \frac{1}{1 + T_+ D_n^+} \right), \]

using independence of \( D_n^+ \) and \( Y_n^+ \). Define

\[ \alpha_+ = E \left( \frac{1}{1 + T_+ D_n^+} \right), \quad \alpha_0 = E \left( \frac{1}{1 + T_0 D_n^0} \right), \]

\[ Q_+ = EQ_+^+ , \quad Q_0 = EQ_0^0 . \]

Then (3a) yields:

\[ (3a') \quad EX_\infty = \frac{T_0 Q_0^0 \alpha_0 + T_+ Q_+^+ \alpha_+}{1 - \alpha_0 \alpha_+} . \]

Similarly,

\[ (3b') \quad EX_\infty = \frac{T_+ Q_+^+ \alpha_+ + T_0 Q_0^0 \alpha_0 \alpha_+}{1 - \alpha_0 \alpha_+} . \]

While equation (2') must be modified if \( D_n^+ \) or \( D_n^0 \) is 0, equations (3a') and (3b') still hold if \( P(D_n^+ = 0) > 0 \) or \( P(D_n^0 = 0) > 0 \). This fact
is verified by showing that \( EB_1 \) still equals \( T_0 Q^O \alpha_o + T^+ Q^+ \alpha_o \alpha_+ \) on the set \( \{(D_1^+ = 0) \cup (D_1^O = 0)\} \).

By Jensen's inequality,

\[
\alpha_+ = E \frac{1}{1 + T^+ D_1^+} > \frac{1}{1 + T^+ \mathbf{ED}_1^+}, \quad \text{and} \quad \alpha_o > \frac{1}{1 + T^+ \mathbf{ED}_1^O}.
\]

Let \( EX^{**}_\infty \) and \( \tilde{E}X^{**}_\infty \) be the results of formula (3a) and (3b) when \( D_1^+ \) and \( D_1^O \) are replaced by their expected values. Then by the above two inequalities:

\[
EX^{**}_\infty \geq EX^{**}_\infty = \frac{T_0 Q^O (1 + T^+ \mathbf{ED}_1^+)}{T_0 \mathbf{ED}_1^O + T^+ \mathbf{ED}_1^+ + T_0 T^+ \mathbf{ED}_1^O \mathbf{ED}_1^+},
\]

and

\[
\tilde{E}X^{**}_\infty \geq \tilde{E}X^{**}_\infty = \frac{T^+ Q^+ (1 + T^+ \mathbf{ED}_1^O)}{T_0 \mathbf{ED}_1^O + T^+ \mathbf{ED}_1^O + T_0 T^+ \mathbf{ED}_1^O \mathbf{ED}_1^+}.
\]

So, \( EX^{**}_\infty \) and \( \tilde{E}X^{**}_\infty \) are underestimated.

Now consider

\[
\int_0^n c(t) dt = \int_0^n \tilde{X}_n \tilde{D}_n^{O} (t - \tilde{t}_n) + Q_n^O \left( 1 - e_n^{O} (t - \tilde{t}_n) \right) dt, \quad \text{for} \quad p_n^O > 0
\]

\[
\tilde{X}_n \tilde{D}_n^{O} (t_n + 1 - \tilde{t}_n) + Q_n^O \left( 1 - e_n^{O} (t_n + 1 - \tilde{t}_n) \right)
\]

\[
= \frac{\tilde{X}_n}{\tilde{D}_n^{O}} (1 - e_n^{O} (t_n + 1 - \tilde{t}_n)) + \frac{Q_n^O}{p_n^O} \left( (t_n + 1 - \tilde{t}_n) - \frac{1}{p_n^O} (1 - e_n^{O} (t_n + 1 - \tilde{t}_n)) \right)
\]

\[
= \frac{\tilde{X}_n}{\tilde{D}_n^{O}} (1 - e_n^{O} (t_n + 1 - \tilde{t}_n)) + \frac{Q_n^O}{p_n^O} (Y_n^O - \frac{1}{p_n^O} (1 - e_n^{O} (t_n + 1 - \tilde{t}_n)))
\]

Now,
\[
\begin{align*}
E\left[\frac{1}{D_n} (Y_n - \frac{1}{D_n} (1 - e^{-D_nY_n}))\right] &= E\{E\left[\frac{1}{D_n} (Y_n - \frac{1}{D_n} (1 - e^{-D_nY_n}) | D_n\right]\} \\
&= E\left\{\frac{1}{D_n} \left(T_0 - \frac{T_0}{1 + T_0D_n}\right)\right\} = T_0^2 \alpha_o .
\end{align*}
\]

So,
\[
E \int_{t_n}^{t_{n+1}} c(t) dt = E \tilde{X}_n T_0 \alpha_o + Q_0 T_0^2 \alpha_o = T_0 E \tilde{X}_n ,
\]

using (3a') and (3b'). This result also holds if \( P[D_n = 0] > 0 \).

Similarly,
\[
\tilde{E} \int_{t_n}^{\tilde{t}_n} c(t) dt = T_+ E \tilde{X}_n .
\]

So,
\[
E \int_{t_n}^{t_{n+1}} c(t) dt = T_0 E \tilde{X}_n + T_+ E \tilde{X}_n .
\]

In a later paper, it will be shown that
\[
\lim_{t \to \infty} Ec(t) = \tilde{c}(\infty) = \lim_{n \to \infty} \frac{E \int_{t_n}^{t_{n+1}} c(t) dt}{E \int_{t_n}^{t_{n+1}} dt} = \frac{T_0 E \tilde{X}_n + T_+ E \tilde{X}_n}{T_0 + T_+} ,
\]

where \( E \tilde{X}_n \) and \( E \tilde{X}_n \) are given in (3a') and (3b').

If \( Q_0 = Q_0 = Q \) and \( D_1 = 1/T_0 \), \( D_1 = 1/T_0 \), then equation 8 on p. 41 of Baker is recovered. Since \( E \tilde{X}_n \) and \( E \tilde{X}_n \) are underestimated by replacing \( D_1 \) and \( D_1 \) by their expected values, \( \tilde{c}(\infty) \) will also be underestimated.
Numerical Example. Consider the example on p. 45 of Baker, where

\[ Q \equiv 1, \quad D_1^0 \equiv 0, \quad D_1^+ = 0.1, \quad T_0 = 50, \quad \text{and} \quad T_+ = 5, \]

which yields \( \bar{c}(\infty) = 150 \). If \( D_1^+ \) actually has density

\[ f_{D_1^+}(x) = 10 \cdot 10^x I_{x > 0}, \]

then \( \overline{ED}_1^+ = 0.1 \), but \( \bar{c}(\infty) = 190 \). So, replacing \( D_1^+ \) by its expected value has caused \( \bar{c}(\infty) \) to be substantially underestimated.

Conclusions. Except for the justification of equation (4), the mathematics used in this paper is quite simple and straightforward, so the technique for computing \( \bar{c}(\infty) \) (the asymptotic expected concentration) is a desirable one. The same method can be used to find higher moments, but the computations would be quite lengthy.

While \( \bar{c}(\infty) \) was computed allowing source and deposition rates to be random, they were still fixed within any one rainy or dry period. Wet deposition is highly dependent on rain intensity, and in the case of sulfur dioxide, on temperature and pH (see Barrie, p. 32). These factors can change significantly during a rainfall, so the assumption that wet deposition is constant during a rainfall may be seriously in error. These calculations made extensive use of the independence of the various factors (source rate, deposition rate, and length of rainy/dry period) within a rainy or dry period, and of their independence from one period to the next. No data have been analyzed to see if these assumptions are reasonable. Also, the problem of estimating the distributions of \( D_1^0 \) and \( D_1^+ \), the random dry and wet deposition rates, has not been dealt with. However, note that all that is needed about \( D_1^0 \) and \( D_1^+ \) to compute \( \bar{c}(\infty) \) are

\[ E\left(\frac{1}{1 + T_0 D_1^0}\right) \quad \text{and} \quad E\left(\frac{1}{1 + T_+ D_1^+}\right). \]

These are both bounded functions, so that
using the empirical distributions of $D_1^0$ and $D_1^+$ will provide consistent estimates of these expectations no matter what the distributions of $D_1^0$ and $D_1^+$ are.

Despite the shortcomings of this model, allowing source and deposition rates to be random is a significant generalization of the result in Baker, especially since replacing the random wet and dry deposition rates by their expected values causes $\bar{c}(\infty)$ to be underestimated.

References
