Calculating Average Airborne Concentrations from and Generation Rates for Emissions for Constant Short-Lived Sources

Susan Arnold, MSOH, CIH, & Mike Jayjock, Ph.D., CIH, The LifeLine Group

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BEYOND THE LIMITS OF CONVENTIONAL ASSESSMENT TOOLS -

- The Challenge

- Estimating generation rates for and average concentrations from constant short term emission rates
Calculating SS Concentrations

Readily available form for calculating well-mixed instantaneous concentrations where $C = 0$ at time $t = 0$:

$$C = \frac{G}{Q} - \frac{G}{Q} e^{-\frac{Qt}{V}}$$

Where:

- $C$ = Concentration (mg/m$^3$)
- $G$ = Constant generation rate (mg/hour)
- $Q$ = ventilation rate (m$^3$/hour)
- $V$ = volume of the box (m$^3$)
- $t$ = time (hours)
Short Term, Task Based Exposures

- Steady State concentrations typically not attained with short term task based exposures

![Graph showing concentration over time]

- Concentration @ 16 minutes = 16.5 mg/m3
- Test Ends @ 16 minutes
Application

- The algorithm for the instantaneous concentration of an agent in a well-mixed room with the initial concentration $C_0 = 0$ and NO contaminant entering with the incoming air is:

$$C = \frac{G}{Q} - \frac{G}{Q} e^{-\frac{Qt}{V}}$$
Contaminant concentration can be estimated for the time period during which the source is emitted by integrating this equation with respect to time – we get the area under the Ct curve:

$$Ct = \frac{G}{Q^2} \left( V + tQe^{\frac{Qt}{V}} \right)e^{-\frac{Qt}{V}} - \frac{VG}{Q^2}$$
Average Concentration for Respective Time Period

- Dividing this $C(t)$ area by the elapsed time gives us the average concentration for that time period.

\[ C_{\text{avg}} = \frac{G}{Q^2} \left( V + tQe^{\frac{Qt}{V}} \right) e^{-\frac{Qt}{V}} - \frac{VG}{Q^2} \]

- *This (Cavg) is, of course, what we measure when we sample.*
Solution for Calculating C and G

- For short term situations in which $G$ is constant over the time interval
- from sources that start at time $t = 0$ and end before or around the elapsed time necessary to achieve $C_{sat}$

$$C_{avg} = \frac{G}{Q^2} \left( V + tQe^{+\frac{Qt}{V}} \right) e^{-\frac{Qt}{V}} - \frac{VG}{Q^2}$$
Solution ‘Portability’

- Solution is useful **and often necessary** for determining G from monitoring data in a well mixed box that has not reached an extended G/Q steady state.
Solution Portability

$$C_{avg} = \frac{G}{Q^2} \left( V + tQe^{\frac{Qt}{V}} \right) e^{-\frac{Qt}{V}} - \frac{VG}{Q^2}$$

expression provides the area under the C,t curve for any period (t) with a starting concentration of zero at \( t=0 \).
Estimating $G_{\text{avg}}$ from $C_{\text{avg}}$

- In any WMR, $C_{\text{avg}}$ – which can be estimated by air sampling, can be used to accurately calculate $G$.

- $C_{\text{avg}}$ can be compared to $C_{\text{eq}}$ (which is always $G/Q$)
  - This assumes that $G$ is constant over time
Comparing Ceq to Cavg

10m$^3$ well mixed Volume with 10 m$^3$/hr Ventilation
(Constant source G = 100 mg/hr starts at t=0)

\[ Ceq = \frac{G}{Q} = 10 \text{ mg/m}^3 \]

Cavg after 30 minutes = 2.1 mg/m$^3$
Generation Rate Portability

\[ G = \frac{C_{\text{avg}} Q^2 t}{V} - \frac{Q t}{Ve} - e^{-\frac{Q t}{V} t} + \frac{Q t}{V} - V \]

- \( G \) determined in this manner can be used in many other models to predict \( C \)
Using G in other models

G determined in this manner is valid for use in any indoor or outdoor exposure model requiring this variable, e.g., 2-Box Model:

\[
C_{\text{NF}}(t) = \frac{G}{Q} + \frac{G}{\beta} + G \left( \frac{\beta \cdot Q + \lambda_2 \cdot V_{\text{NF}} (\beta + Q)}{\beta \cdot Q \cdot V_{\text{NF}} (\lambda_1 - \lambda_2)} \right) \exp (\lambda_1 \cdot t) - G \left( \frac{\beta \cdot Q + \lambda_1 \cdot V_{\text{NF}} (\beta + Q)}{\beta \cdot Q \cdot V_{\text{NF}} (\lambda_1 - \lambda_2)} \right) \exp (\lambda_2 \cdot t)
\]

Where

\[C = \text{Concentration (mg/m}^3)\]
\[G = \text{Constant generation rate (mg/hour)}\]
\[Q = \text{ventilation rate (m}^3\text{/hour)}\]
\[V_{\text{NF}} = \text{volume of the inner box or Near Field (m}^3)\]
\[V_{\text{FF}} = \text{volume of the outer box or Far Field (m}^3)\]
\[\beta = \text{Interzonal airflow (m}^3\text{/hour)}\]
\[t = \text{time (hours)}\]
Using G in other models

- e.g. Eddy Diffusivity Concentration Models

\[
C(r, t) \equiv \frac{G}{2 \cdot \pi \cdot D_T \cdot r} \cdot \left[ 1 - \sqrt{1 - \exp\left( -\frac{r^2}{\pi \cdot D_T \cdot t} \right)} \right]
\]

- Where
  - \( C(r, t) \) = Concentration (mg/m\(^3\))
  - \( G \) = Constant generation rate (mg/hour)
  - \( D_T \) = Eddy Diffusion Coefficient (m\(^3\)/hour)
  - \( t \) = time (hours)
- Assumes: hemispherical diffusion from a point source on the ground.
Using G in other models

- Both models require G to estimate C
  - G determined in this manner is the same and relevant; which is very useful in looking at other scenarios, conducting research or estimating exposure.
In Summary

- Useful in research and modeling
- One way of indirectly measuring $G$
- For passive volatilization or vessel filling displacement of a volatile or semi-volatile organic compound, physical chemical principals could also be used to estimate $G$

- However, for constant particulate emission sources, the methodology described herein may be the only reasonable option for estimating $G$. 