

### Vapor Scavenging Coefficient Estimation

Vapor scavenging coefficients are used to estimate the rate of removal of a soluble species that exists below the cloud line based on rain event characteristics, such as intensity and droplet size. This section explains the technical basis for the estimation of the scavenging coefficient of C-8 out of the vapor phase. The basis for this estimation is provided in "Atmospheric Chemistry and Physics" by J.H. Seinfeld and S.M. Pandis (1998, Wiley & Sons).

Two key assumptions have been made for the purposes of this estimation. First, we have assumed C-8 is irreversibly absorbed into the rain droplet. This is a reasonable assumption in this case, since the C-8 concentration in the droplet would be low and the C-8 would almost certainly be dissociated and therefore non-volatile. Second, while Seinfeld steps through a derivation for scavenging coefficients for a specified droplet size, it is much more accurate a determination to include a more representative spectrum of droplet sizes. This assumption will be discussed in more detail below.

The scavenging coefficient for an irreversibly soluble gas by definition is

$$\Lambda = \int_0^{\infty} (\pi * D_p^2 * K_c * n) dD_p$$

where  $D_p$  is the diameter of the raindrop (cm),  $K_c$  is the mass transfer coefficient of a gaseous molecule to a sphere and  $n$  represents some raindrop size distribution relationship.

The mass transfer coefficient,  $K_c$ , can be calculated by empirical correlations, such as

$$K_c = \frac{D_g}{D_p} \left[ 2 + 0.6 * \left( \frac{\rho_{air} * U_t * D_p}{\mu_{air}} \right)^{1/2} * \left( \frac{\mu_{air}}{\rho_{air} * D_g} \right)^{1/3} \right]$$

where  $D_g$  is the gas phase diffusivity of the species (cm<sup>2</sup>/sec),  $U_t$  is the droplet velocity (cm/sec),  $\rho_{air}$  is the density of air (g/cm<sup>3</sup>) and  $\mu_{air}$  is the viscosity of air (g/cm-sec). The gas phase diffusivity of the C-8 molecule was estimated to be 0.0423 cm<sup>2</sup>/sec by the method of Fuller et al. Droplet velocity is a function of raindrop particle diameter,  $D_p$ , and for the purposes of this estimation, was estimated by a curve-fit of data from Table 20.1 (page 1006) of Seinfeld's book, and expressed as

$$U_t = 1041.7 * \sqrt{D_p}$$

The raindrop size distribution,  $n$ , as described by Marshall and Palmer (1948) is commonly used in estimating scavenging coefficients. According to the authors, this relationship may overestimate by as much as 50% the number of small droplets in the 0.02 to 0.12 cm size range, thus causing a conservative estimate of the scavenging coefficient. The relationship is expressed as

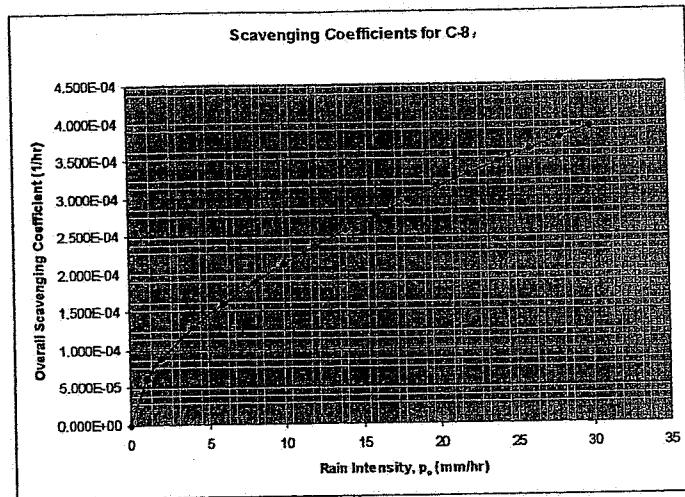
$$n = 0.08 * \exp\{-41 * D_p * p_o^{-0.21}\}$$

where  $p_o$  is the rain intensity (mm/hr).

Substitution of the expressions for  $K_c$ ,  $U_t$ , and  $n$  into the scavenging coefficient equation yields an integral expression that is difficult to integrate explicitly. For the purposes of this estimation, the final expression was numerically integrated between raindrop particle sizes of 0 and 1 cm. An upper limit of 1 cm was chosen because it represents a reasonable maximum raindrop size, beyond which the raindrop will break apart into smaller droplets that are < 1cm.

Results of the numerical integration are shown below in tabular and graphical form. The maximum intensity value used was 30 mm/hr, which exceeded the maximum observed intensity of 27.9 mm/hr recorded at the Washington Works site.

| Rain Intensity<br>(mm/hr) | Scavenging<br>Coefficient |
|---------------------------|---------------------------|
| 0                         | 1.352E-09                 |
| 1                         | 5.974E-05                 |
| 2                         | 8.767E-05                 |
| 4                         | 1.286E-04                 |
| 6                         | 1.610E-04                 |
| 8                         | 1.887E-04                 |
| 10                        | 2.135E-04                 |
| 12                        | 2.362E-04                 |
| 14                        | 2.573E-04                 |
| 16                        | 2.771E-04                 |
| 18                        | 2.959E-04                 |
| 20                        | 3.137E-04                 |
| 22                        | 3.308E-04                 |
| 24                        | 3.472E-04                 |
| 26                        | 3.630E-04                 |
| 28                        | 3.782E-04                 |
| 30                        | 3.931E-04                 |



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