Volatilization Alternative explanation

Transport processes, including volatilization, leaching, lateral mass flux are considered sequentially before degradation and direclty after application. Sorption is considered within each process.

Volatilization

Volatilization is assumed only to take only place on the application day, and follows Leistra et al. [2001] by considering mass flux across two boundary layers. Mass flux across an air boundary $J_{v,a}$ $(\mu g/m^2 d)$ and mass flux across the top soil layer $J_{v,s}$ $(\mu g/m^2 d)$ and given by:

$$.J_{v,air} = \frac{-(C_{g,0(t)} - C_{air})}{r_{air(t)}}$$

$$.J_{v,soil} = \frac{-(C_{g,z0} - C_{g,0})}{r_{soil(t)}}$$

where, r_a (d/m) is the air boundary resistance and r_s (d/m) the top soil layer resistance before the pesticide reaches the soil surface from the center of the cell layer $(0.5 \cdot D_{z0})$. Concentration gradients $(\mu g/m^3)$ are considered based on the concentration at the soil surface $C_{g,0}$, the air boundary layer C_{air} and at the center of top soil layer.

Resistance across the boundary air and soil layers are given respectively by:

$$.r_{air(t)} = \frac{D_{z,air}}{D_{a(t)}}$$

$$.r_{soil(t)} = \frac{0.5 \cdot D_{z0}}{D_{diff,g}}$$

where $D_{z,air}$ (m) is the boundary air layer assumed to be equal to the the first soil layer $(k = z0)$ thickness and the pesticide diffusion coefficient D_a (m^2/d), which is dependent on the daily air temperature T (in K) as:

$$.D_{a(t)} = \left(\frac{T}{T_r}\right)^{1.75} D_{a,r}$$

and where $D_{a,r}$ (m^2/d), is the diffussion coefficient in air at reference temperature T_r. Two options are available to compute the relative diffusion coefficient $D_{diff,g}$ (m^2/d), which is adjusted to the available pore air space $\theta_{z0,air(t)} = \theta_{z0,sat} - \theta_{z0(t)}$. The first option is given by [Millington and Quirk, 1960, Jin and Jury, 1996]:

$$.D_{diff,g(t)} = \frac{D_{a(t)} \cdot (\theta_{z0,air(t)})^2}{(\theta_{z0,sat})^{2/3}}$$

The second option is given by [Currie, 1960, Bakker et al., 1987]:

$$.D_{diff,g(t)} = 2.5 \cdot D_{a(t)} \cdot (\theta_{z0,air(t)})^3$$

During each process, sorption extent is computed (as shown above) to obtain the concentration in aqueous $C_{z0,aq}$ $(\mu g/L)$ and gas $C_{z0,g}$ $(\mu g/L)$ solutions. It is assumed that the diffusion flux from the top soil layer is equal to the diffusion flux across the bounadry air layer and that concentration in air $C_{air} = 0$, yielding:

$$C_{g,0} = \frac{r_{air(t)}}{r_{air(t)} + r_{soil(t)}} \cdot C_{g,z0} \tag{1}$$

Substituting eq. 1 into **??** ...

The volatilized flux out of the top layer is given by:

...this has been documented in BEACH Methodoogy!!

References

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