

Calculation of time weighted average concentrations with mkin

Johannes Ranke

2017-03-28

Since version 0.9.45.1 of the ‘mkin’ package, a function for calculating time weighted average concentrations for decline kinetics (*i.e.* only for the compound applied in the experiment) is included.

Time weighted average concentrations for the DFOP model are calculated using the formulas given in the FOCUS kinetics guidance (FOCUS Work Group on Degradation Kinetics 2014, 251):

SFO:

$$c_{\text{twa}} = c_0 \frac{(1 - e^{-kt})}{kt}$$

FOMC:

$$c_{\text{twa}} = c_0 \frac{\beta}{t(1 - \alpha)} \left(\left(\frac{t}{\beta} + 1 \right)^{1 - \alpha} - 1 \right)$$

DFOP:

$$c_{\text{twa}} = \frac{c_0}{t} \left(\frac{g}{k_1} (1 - e^{-k_1 t}) + \frac{1 - g}{k_2} (1 - e^{-k_2 t}) \right)$$

Often, the ratio between the time weighted average concentration c_{twa} and the initial concentration c_0

$$f_{\text{twa}} = \frac{c_{\text{twa}}}{c_0}$$

is needed. This can be calculated from the fitted initial concentration c_0 and the time weighted average concentration c_{twa} , or directly from the model parameters using the following formulas:

SFO:

$$f_{\text{twa}} = \frac{(1 - e^{-kt})}{kt}$$

FOMC:

$$f_{\text{twa}} = \frac{\beta}{t(1 - \alpha)} \left(\left(\frac{t}{\beta} + 1 \right)^{1 - \alpha} - 1 \right)$$

DFOP:

$$f_{\text{twa}} = \frac{1}{t} \left(\frac{g}{k_1} (1 - e^{-k_1 t}) + \frac{1 - g}{k_2} (1 - e^{-k_2 t}) \right)$$

FOCUS Work Group on Degradation Kinetics. 2014. *Generic Guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in Eu Registration*. 1.1 ed. <http://focus.jrc.ec.europa.eu/dk>.