

Implementation of bi-phasic kinetics for 1,2,4-triazole in PEARL/GeoPEARL

Background

For 1,2,4-triazole (a metabolite formed from several triazole fungicides) endpoints were agreed at PRAPeR 12 meeting of 15 – 18 January 2007. The Triazole Derivative Metabolite Group (TDMG) has submitted additional field dissipation data for 1,2,4-triazole as part of confirmatory data requirements, which resulted in a revision of the DT₅₀ values to be used in FOCUS modelling (proposed revision to DT₅₀ for 1,2,4-triazole (July 2011, revised September 2011 and January 2013)).

Instructions for modelling

TDMG submitted new field dissipation data for 1,2,4-triazole demonstrating bi-phasic degradation (DFOP): geomean normalised field DT₅₀ (n=4): DT₅₀ (fast phase) = 1.68 d; DT₅₀ (slow phase) = 60.5 d; arithmetic mean g-value = 0.489

In section 7.1.2.2.2 of FOCUS Kinetics a higher tier approach is described for implementation of bi-phasic kinetics for 1,2,4-triazole in pesticide leaching models. For metabolites the same approach is recommended in section 8.3.3.2.2. In Appendix 5 the method is described in more detail. Here it is stated that the simulation is strictly correct only when the Freundlich exponent is one (linear isotherm). However, a conservative estimate can be made when the Freundlich exponent is not one by doubling the application rate and then dividing the final answer by two. In the case of 1,2,4-triazole the mean 1/n is 0.916. Therefore the “application rate” for 1,2,4-triazole should be doubled. However, the Guidance is silent about the way to double the “application rate” for metabolites. When a simulation is performed in which the transformation scheme is used, doubling the application rate of the parent will not necessarily lead to a doubling of the amount of 1,2,4-triazole formed in the simulation. This is due to the fact that the parent, and possible other predecessors, are subject to several loss processes which are not linear. The only way to ensure that the amount of 1,2,4-triazole is doubled, is to perform a simulation in which 1,2,4-triazole is modelled as parent. However, this kind of modelling, disregarding the transformation scheme, may lead to an underestimation of the leaching.

Therefore both simulations has to be performed in a risk assessment in order to establish which method calculates the highest concentrations for 1,2,4-triazole on a case-by-case basis.

Simulation following transformation scheme (1 run sufficient per application scheme):

- application rate of the parent is doubled;
- 1,2,4-triazole is included in the scheme using two compartments (fast and slow degradation phase);
- fast phase DT₅₀ value of 1.68 d used for the fast degrading compartment;
- slow phase DT₅₀ value of 60.5 d used for the slow degrading compartment;
- formation fraction of fast degrading compartment: formation fraction* x 0.489;
- formation fraction of slow degrading compartment: formation fraction* x (1-0.489);
- calculated overall 80th percentile (PEARL) or 90th percentile (GeoPEARL) concentrations of the fast and slow degrading compartment need to be summed and divided by two**.

Simulation with 1,2,4-triazole modelled as parent (2 runs required per application scheme):

- one simulation run for the fast degrading compartment (DT₅₀ 1.68 d) using a doubled application rate corrected for molecular weight and the proportion of flow from precursor to the fast degrading compartment:
2 x application rate (kg/ha) x (69.1/mol.weight parent) x (formation fraction* x 0.489);
- one simulation run for the slow degrading compartment (DT₅₀ 60.5 d) using a doubled application rate corrected for molecular weight and the proportion of flow from precursor to the slow degrading compartment:
2 x application rate (kg/ha) x (69.1/ mol.weight parent) x (formation fraction* x (1-0.489));

- calculated overall 80th percentile (PEARL) or 90th percentile (GeoPEARL) concentrations of the fast and slow degrading compartment need to be summed and divided by two**.

* the new DT₅₀ values are derived from field studies with 1,2,4-triazole dosed as parent. Therefore, these new endpoints cannot be combined with a formation fraction (or max. obs.%) from a laboratory study. In principle they can be combined with a formation fraction (or max. obs.%) from a field study in which the parent was dosed. However, as for most triazole fungicides only the parent will have triggered field studies, it is not likely that a formation fraction (or max. obs.%) is available for 1,2,4-triazole. Therefore in most cases a worst case formation fraction of 1 should be used in the modelling.

** in principle the summing of the concentrations of the fast and slow degrading compartment and subsequent division should be done for each time step of the model (i.e. one day). The 80th/90th percentile should then be calculated based on these results. However, as the concentrations for each time step are not readily available as output, the overall 80th/90th percentile is used. In this case this is acceptable as only the slow degrading compartment contributes to the calculated leachate concentration. Therefore, division by two of the concentrations of the slow degrading compartment for each time step will not differ from the division by two of the overall 80th/90th percentile.