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OFFICE OF PREVENTION, PESTICIDES AND TOXIC SUBSTANCES

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MEMORANDUM: Calculation of Half-lives of RPA 202248 in Aerobic Soil Metabolism Study (MRID 43588006) for Isoxaflutole and EEC's for Surface and Ground Water

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General Conclusions

Previous estimates of the half-lives of the isoxaflutole metabolite RPA 202248 in aerobic soil (MRID 43588006) involved linear regression using log-transformed data, and either did not use all the data points or did not provide half-lives that were representative of the data. EFED recalculated the half-lives of RPA 202248 in aerobic soils to achieve more representative estimates of persistence that used all the data points. This was accomplished using the Optimizer tool in Quattro Pro to do a non-linear regression using untransformed data. The settings on the Optimizer were central estimations of derivatives and automatic scaling. The model fit the raw data well, with R^2 values of 0.95 for both the sandy loam and clay soils (See Table 1 below). Tables 2 and 3 present the EEC's for ground and surface water, respectively, calculated with each of the half-lives.

First-order kinetics is not the best model, based on significant lack of fit. When this is the case, the regular linear regression provides a poor estimate of the rate constant for use in modeling. EFED used non-linear regression on untransformed data because it provides a better description of the kinetics for use in modeling. It allows the reviewer to account for all the data in a calculation of the estimated half-life.

The inputs for this model included the percent of nominal as a function of time, from which the degradation rate of parent isoxaflutole, the presence (or absence) of any competing degradation

parent isoxaflutole and RPA 202248 were calculated. The model predicted concentrations of RPA 202248 in aerobic soil. The observed values and the difference between the observed and predicted concentrations of RPA 202248 (residuals) were squared and put into separate columns in the spreadsheet. The formation constant of RPA 202248 was set to be $\leq$ the degradation rate constant of parent isoxaflutole. If the formation constant of RPA 202248 was equal to the degradation rate constant of parent isoxaflutole, then no competing processes were considered to be present.

To reduce ground water contamination concerns, the registrant has modified the proposed label to prevent use on many sandy soils. The resulting label is extremely large and is not user friendly or very practical.

Table 1. Summary Table for Outputs of Linear and Non-Linear Models for Sandy Loam and Clay Soils as Calculated by EFED and the Registrant.

Soils/	Source (EFED or Registrant)	Half-life (days)	R^2	F/Probability	Time Interval used in Calculations
Sandy Loam (linear)	Registrant	20	0.88	14.5/6.2e-2	7-63 days
Sandy Loam (linear)	EFED	115	0.59	13.7/6e-3	7-365 days
Sandy Loam (non-linear)	EFED	17	0.95	96/1.1e-7	0-365 days
Clay (linear)	Registrant	37	0.96	55/1.8e-2	7-63 days
Clay (linear)	EFED	186	0.66	13.8/7.6e-3	7-365 days
Clay (Non-linear)	EFED	61	0.95	116/4e-8	0-365 days

Table 2. EEC's in Ground Water with Calculated Half-Lives, Application Rate of 0.14 lbs ai/A, and K_{oc} of 92 as Inputs.

Half-life (days)	Ground Water EEC's using SCI-GROW2 for use in Acute, Chronic, and Cancer Risk Asessment (ug/L)
17	0.02
61	0.11
106*	0.23
115	0.26
186	0.46

*106 days was upper 90th percentile of 17 and 61 days. This half-life was used to generate EEC's in the Dietary Risk Assessment sent to HED.

Table 3. Tier II upper tenth percentile EEC's for RPA 202248 for simulated corn using PRZM 2.3 and EXAMS 2.94. All EEC's are **one-in-ten year** values except for the long-term means.

Aerobic Soil Metabolism Half-Life	Maximum ($\mu g \cdot L^{-1}$) **(1-in-10 year mean)**	4 Day ($\mu g \cdot L^{-1}$) **(1-in-10 year mean)**	21 Day ($\mu g \cdot L^{-1}$) **(1-in-10 year mean)**	60 Day ($\mu g \cdot L^{-1}$) **(1-in-10 year mean)**	90 Day ($\mu g \cdot L^{-1}$) **(1-in-10 year mean)**	Annual Mean* ($\mu g \cdot L^{-1}$) **(1-in-10 year mean)**	Long-Term Mean* ($\mu g \cdot L^{-1}$) **(Student's upper 90th percentile confidence bound of the annual means from the PRZM run)**
17 days	1.7	1.7	1.7	1.7	1.7	1.5	1.1
61 days	2.0	2.0	2.0	2.0	1.9	1.7	1.3
106 days	2.0	2.0	2.0	2.0	1.9	1.7	1.3
115 days	2.1	2.1	2.1	2.0	2.0	1.8	1.3
186 days	2.2	2.2	2.2	2.1	2.1	1.9	1.4

* Upper 90% confidence bound on the 36 year mean with the variance calculated from the annual means.