Aqueous Photolysis of [test compound]

|  |  |
| --- | --- |
| Report: | [Provide full citation. Provide the MRID (first) if the review is unilateral.] |
| Document No.: | [MRID xxxxxxxx] |
| Guideline: | OCSPP 835.2240[If the study was conducted under a different guideline, state ‘Conducted by’ and provide the most relevant guideline(s) the study was conducted under. Then state ‘Reviewed by OCSPP 835.2410.’ If this review is multilateral, also provide the guideline numbers under which participating agencies are reviewing the study.] |
| Statements: | [Indicate whether the study was conducted in compliance with FIFRA GLP standards and whether signed and dated Data Confidentiality, GLP Compliance, Quality Assurance, and Authenticity Certification statements were provided. If the study was not conducted in compliance with FIFRA GLP standards, indicate how not or why not.] |
| Classification: | This study is [provide classification and very concise statement of any deficiencies that impacted the classification]. [If multiple classification terminologies are needed for multilateral reviews, list or tabulate them.] |
| PC Code: | [xxxxxx] |
| Reviewer: | [Provide final reviewer(s)’s name Signature:and title.] Date: [Type date of signature.] |

**Executive Summary**

In an aqueous photolysis study, the phototransformation of [[type of radiolabel(s)]-labeled[test compound] was investigated in [sterile aqueous buffered solutions at pH # (buffer used)] at [x] ± [x] ºC using [light source] for a period of [x] days (equivalent to [x] days natural summer sunlight at 40 ºN). Test and control soil samples were treated at [test concentration] mg a.i./kg, which is equivalent to a field application rate of [#] g a.i./ha ([#] lbs a.i./a). A control experiment was conducted under the same experimental conditions except the control samples were kept in the dark (absence of light). Duplicate samples were collected and analyzed using [methods used (*e.g.*, LSC and HPLC-UV].

The phototransformation profile of [test compound] was [similar/different] for both irradiated and control samples indicating. [Add a brief sentence to explain the pattern of degradation. If the phototransformation is not first order, additional discussion is needed.] The overall mass balance for the study ranged from [# to #]. The test system [was/was not] adequate to trap both organic and inorganic volatile compounds. CO2 accounted for up to [x]% of applied radioactivity. Other volatile compounds accounted for [#]% of the applied radioactivity. Major phototransformation products included [x], [y], and [z]. The observed DT50 for the phototransformation of [test compound] was [#] days. The calculated dark control-adjusted DT50 for the phototransformation of [test compound] under summer sun at 40 °N latitude was [#] days. More information on the phototransformation of [test compound] is provided in **Table 1**. [If the environmentally relevant half-life cannot be calculated, include a brief summary of why it cannot be calculated. Include a brief description of how the estimated and observed DT50 values compare and state the best fit model used.]

The duration of the experiment was [not adequate/adequate] to observe the formation and decline of the transformation products. [If a natural water source was used, explain the relevance and usefulness of the data.] The calculated DT50 values for the major transformation product(s) [name(s) here] ranged from [#] to [#] days, respectively.[[1]](#footnote-1)

**Table 1. Results Synopsis: Aqueous Phototransformation of [Test Compound]**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound Name | Observed DT50 (hours/days) | Observed DT90(hours/days) | SFO Half-life A (hours/days) | Model Parameters and Statistics | **Adjusted Half-life (days) B** | **Phototransformation Products**(Common Name (maximum %AR C observed, associated interval)) |
| **Major** | **Minor Identified** |
| **Irradiated: [buffer or natural water, pH #, # °C]** |
| Parent [test compound] | [#] | [#] | [#] | C0=[#], k=[#], SSFO=[#], r2=[#], p=[#] | **[#]** | [name] (# %, # days) | [name] (# %, # days) |
| [Transformation product]\* | [#] | [#] | [#] | C0=[#], k=[#], SSFO=[#], r2=[#], p=[#] | **[#]** | [name] (# %, # days) | [name] (# %, # days) |
| A The Single First-Order (SFO) kinetics model is used to describe abiotic photolytic degradation.B Dark control-adjusted and adjusted to a 12-hour/day photoperiod at 40 °N latitude.C AR means “applied radioactivity.”[If the experiment permits half-life calculations for phototransformation products, include the information in this table.] |

**I. Material and Methods**

**A. Materials:**

**1. Test Material:** [[Type of radiolabel]-labeled[test compound]
Specific radioactivity: [value; units]

 Radiochemical purity: [percentage (HPLC, TLC)]

 Chemical purity: [percentage (HPLC)]

 Batch number: [value]

 Solubility in water: [value] mg/L [If pH-dependent, list available values at each study pH.]

**2. Reference** [List the common name and batch number of each reference

**Compounds:** compound. Provide other chemical information in the structure table.]

**3. Test Media:** [Describe buffered solutions of natural water used in experiments]

Table 2. Physicochemical Properties of [media] used in photolysis study

|  |  |
| --- | --- |
| Property | Reported Value |
| pH | [#] |
| Electrical Conductivity (µS/cm) | [#] |
| Total Carbon (mg/L) | [#] |
| Total Inorganic Carbon (mg/L) | [#] |
| Total Suspended Solids (mg/L) | [#] |
| Nitrate-Nitrogen (mg/L) | [#] |
| Ammonium-Nitrogen (mg/L) | [#] |
| Alkalinity as HCO–3 (mg/L) | [#] |
| Total Magnesium (mg/L) | [#] |
| Total Calcium (mg/L) | [#] |
| Total Iron (mg/L) | [#] |
| Total Dissolved Iron (mg/L) | [#] |
| Ferric Ion Concentration (mg/L) | [#] |
| Ferrous Ion Concentration (mg/L) | [#] |

**B. Study Design:**

1. **Experimental Conditions:**

[If molar absorptivity was investigated and reported in the study report include the methods used and reference the tiered experimental design.]

Table 3. Experimental Design

|  |  |  |
| --- | --- | --- |
| **Parameter** |  | Description |
| Nature of light source  |  |  |
| Emission wavelength spectrum  |  |  |
| Nominal light intensity  |  |  |
| Filters used  |  |  |
| Relationship to natural sunlight  |  |  |
| Method used to determine relations between light source and summer sunlight (*e.g.*, 40 ºN) |  |  |
| Duration of the test |  |  |
| Solution volume |  |  |
| Sterilization method |  |  |
| Test concentration (µg ai/L) |  |  |
| Control conditions |  |  |
| Number of replicates | Irradiated |  |
|  | Darkness |  |
| Test apparatus | Irradiated |  |
|  | Darkness |  |
| Traps | Organics |  |
|  | CO2 |  |
| Test material application | Solvent |  |
|  | Test solution volume used/ treatment |  |
|  | Application method |  |
|  | Evaporation of application solvent |  |
| Indication of test material adsorbing to walls of test apparatus |  |  |
| Experimental conditions | Temperature (°C) |  |
|  | Continuous irradiation |  |
|  | Moisture content |  |
|  | Moisture maintenance method |  |
|  | Continuous darkness (Yes/No): |  |
| Sample storage before analysis |  |  |

1. **Description of Analytical Procedures:**

Samples were analyzed using [LSC] for determination of total radioactivity. [Reversed-phase HPLC with 14C-flow-through detection techniques and normal phase TLC] were used as primary and confirmatory chromatographic methods for the separation and quantitation of products formed. The limit of detection (LOD) was determined to be [percentage] of the applied radioactivity (%AR), with a limit of quantitation (LOQ) at [percentage]AR.

**II. Results and Discussion**

[If molar absorptivity was investigated and reported in the study report, include the results of the study here referencing the tiered experimental design.]

1. **Data:**

Table 4. Aqueous Photodegradation of [radiolabel-test compound] expressed as percentage of applied radioactivity [Add to the table as needed for additional media such as natural water. The results including total mass balances and distribution of radioactivity are presented as individual replicate values rather than means and standard deviations.]

|  |  |
| --- | --- |
|   | Percent of Applied Radioactivity |
| Sampling Interval (hours) | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| Replicate | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| Component | Irradiated [media, pH #, # °C] |
| [Test compound] | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| [Degradate 1] | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| [Degradate 2] | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Unidentified | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Volatiles | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14CO2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Mass Balance | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Sampling Interval (hours) | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| Replicate | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| Component | Control (Dark)[media, pH #, # °C] |
| [Test compound] | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| [Degradate 1] | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| [Degradate 2] | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Unidentified | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Volatiles | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14CO2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Mass Balance | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Data obtained from [Table #, pp. #] of the study report.Total Characterized Residues is the sum of identified and unidentified extractable residues and volatilized compounds.n.d. = not detected, n.a. = not analyzed |

1. **Mass Balance:**

Recoveries ranged from [percentage] to [percentage]AR for the irradiated experiment and [percentage] to [percentage]AR for the control experiment. [Indicate whether there was substantial loss of radioactivity by sorption to glassware or volatilization. Indicate whether a substantial amount of radioactivity was unidentified.]

1. **Volatilization:**

Volatiles [were/were not] trapped. The level of CO2 evolved was [#]%.[Add information regarding additional volatile chemical as need.]

1. **Transformation of Test Compound:**

Degradation of [radiolabel-test compound] in water was [gradual, rapid, or some other characterization]. The DT50 ranged from [x] to [x] as highlighted in **Table 5**. [Indicate the software used to determine model parameters. Indicate whether reviewer-reported half-lives are consistent with study-reported values and the relationship between calculated and observed values. If multiple experiments were conducted per study condition such as using two different test compounds (*i.e.*, different radiolabels), calculate kinetic values for combined data. Discuss any abnormalities observed in the data.]

[Images of kinetics calculation results using the R program may replace most of **Table 5** (dark-control adjusted half-lives and environmental half-lives would still need to be reported). R images should include the model parameters and statistics that are otherwise reported in **Table 5**.]

**Table 5. Aqueous Phototransformation of [Test Compound]** A

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Compound Name | Observed DT50 (hours/days) | Observed DT90(hours/days) | **Calculated****Half-life** B **(days)** | **SFO Model Parameters** B | **SFO Model Statistics** | **Dark Control Adjusted Half-life (days) C** | **Environmental** **Half-life (days) C** |
| Parent [test compound] | [#] | [#] | [#] | C0=[#], k=[#] | SSFO=[#], r2=[#], p=[#] | **[#]** | **[#]** |
| Control: Parent [test compound] | [#] | [#] | [#] | C0=[#], k=[#] | SSFO=[#], r2=[#], p=[#] |  |  |
| Degradate [compound]\* | [#] | [#] | [#] | C0=[#], k=[#] | SSFO=[#], r2=[#], p=[#] | **[#]** | **[#]** |
| Control: Degradate [compound]\* | [#] | [#] | [#] | C0=[#], k=[#] | SSFO=[#], r2=[#], p=[#] |  |  |
| A Data were obtained from [location of data in study report] and calculations in the attached Excel workbook [name(s) of worksheets, if needed]. See Attachment 3 for calculations.B The Single First-Order (SFO) kinetics model is used to describe abiotic photolytic degradation.C Half-life value was adjusted to a 12-hour/day photoperiod under summer sun at 40 °N latitude).  |

[Half-lives should be calculated with non-linear regression assuming single first-order (SFO) kinetics and following the NAFTA kinetics guidance (USEPA, 2011). Other half-life calculation methods may be added to the table when needed, such as when degradation is not first-order. Rows may be added for transformation product half-lives and DT50s as needed. If multiple experiments were conducted per study condition using test compound with different radiolabel positions, calculate kinetics values for the combined data rather than for specific radiolabeled positions.]

[Briefly summarize the transformation products per system in Table 6. If transformation product decline is observed over four time intervals, calculate a half-life and discuss the pattern of decline. Based on the control experiment, discuss which transformation products are the likely result of phototransformation as compared to other degradation processes.]

**Table 6. Transformation Products of [Test Compound] in Water**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Transformation Product(s) | Maximum %AR Observed | Associated Interval | Final %AR Observed | Final Interval |
| Irradiated Samples | [common name] | [#] | [# d] | [#] | [# d] |
| [common name] | [#] | [# d] | [#] | [# d] |
| Controls | [common name] | [#] | [# d] | [#] | [# d] |
| [common name] | [#] | [# d] | [#] | [# d] |

 [If applicable, provide a description of the transformation pathway here, including a schematic as Figure 1.]

**[Figure 1. Aqueous Phototransformation Pathway of [radiolabel-test compound]]**

1. Findings:

[Include the result of any checks on pH, sterility, or other test condition. Don’t repeat information in the executive summary. If no additional information is needed refer to the Executive Summary]

**III. Study Deficiencies and Reviewer’s Comments**

[This section is titled “Conclusions” in the original T2S template.]

[List any deficiencies with the study and any additional salient information. Results and conclusions contained in the Executive Summary are not repeated in this section.]

**IV. References** [List any references cited in the review.]

U.S. Environmental Protection Agency (USEPA). 2011. Guidance for Evaluating and Calculating Degradation Kinetics in Environmental Media. (Interim draft document dated Dec. 21, 2011.)

**Attachment 1: Chemical Names and Structures**

[A table (*i.e.*, structure table) of the chemical names, SMILES strings, CAS numbers, and structures of the test compound, all identified transformation products, and all reference compounds that were not identified in study samples should be either referenced as a separate, associated document or attached to the study review. Multiple versions of structures to show or not show radiolabeling and multiple versions of chemical names and SMILES strings should not be included in the table. Sources of data need not be included. However, formatting the structure table in conformance with the guidance for tabulating transformation product data for EFED ROCKS memoranda is recommended. This formatting includes table columns for MRIDs and associated study data such as maximum and final concentrations of transformation products and their intervals.

For multilateral reviews, chemical names, SMILES strings, structures, and CAS numbers are captured elsewhere in the Monograph[[2]](#footnote-2). Therefore these data are not attached to each study review within the Monograph. When the Monograph is split into individual reviews in EFED’s files, however, the Monograph’s structure table should be either referenced as a separate, associated document or attached to each individual review.]

[Sample structure table with the minimum information needed.]

|  |
| --- |
| **[Common name [list other common names] [if the same common name is used in different studies for different compounds, provide in parentheses the MRID associated with the common name for this compound.]]** |
|  |  |
| IUPAC Name: | [Provide one IUPAC name.] |
| CAS Name: | [Provide one CAS name.] |
| CAS Number: | [Provide if available.] |
| SMILES String: | [Provide one SMILES string.] |
|  |
| [Paste structure here.] |
|  |
|  |

[Sample EFED ROCKS memorandum format for structure tables.]



Attachment 2: Statistics Spreadsheets and Graphs



[Supporting electronic spreadsheet files should be inserted here (electronic attachment files should be electronically finalized as separate files as well). Electronic attachments should have the same file name as the Microsoft Word study review file with the addition of “Calc” for Excel workbooks and WinZip files, the addition of “Data” for Adobe Acrobat and Document Imaging files, and the addition of brief descriptors as appropriate for SigmaPlot Notebooks. Electronic attachment files should be compressed into a WinZip file when three or more are prepared for a study review.]

[Hard copies of a study review and any attachment sheets from separate electronic files should be printed and finalized together as one hard copy file.]

Attachment 3: Calculations

Calculations were performed by the reviewer using [indicate program(s) used for calculations] and the following equations. [The following equations are anticipated to reflect the NAFTA kinetics guidance as of January 2012. If these equations are not current, they should be replaced by the applicable equations from current guidance.]

Single First-Order (SFO) Model

$C\_{t}=C\_{0}e^{-kt}$ (eq. 1)

where,

 Ct = concentration at time t (%)

 C0 = initial concentration (%)

 e = Euler’s number (-)

 k = SFO rate constant of decline (d-1)

 t = time (d)

The SFO equation is solved [with the Excel Solver] by adjusting *C0* and *k* to minimize the objective function (SSFO) shown in equation 4.

DT50 = natural log (2)/k (eq. 2)

DT90 = ln (10)/k (eq. 3)

$S\_{SFO}=\sum\_{}^{}(C\_{model},t-C\_{d,t})^{2}$ (eq. 4)

where,

SSFO = objective function of SFO model fit (%2)

n = number of data points (-)

Cmodel,t = modelled value at time corresponding to Cd,t (%)

Cd,t = experimental concentration at time t (%)

1. [Calculate the half-life values for transformation products based on the maximum amount of the transformation product observed and its decline over at least four sampling intervals. Simultaneous formation and decline of the transformation product was not accounted for in the calculation or discuss how it was taken into account.] [↑](#footnote-ref-1)
2. A Monograph is a collection of multiple study reviews and data summaries prepared by government agencies into a single document that follows an OECD format. Typically, Tier II Summaries prepared by industry are updated by government agencies based on agency-review and then placed within the Monograph. [↑](#footnote-ref-2)