Aerobic (or Anaerobic) Degradation in Soil of [test compound]

|  |  |
| --- | --- |
| Report: | [Provide full citation. Provide the MRID (first) if the review is unilateral.] |
| Document No.: | [MRID ########] |
| Guideline: | [OCSPP 835.4100 (aerobic) or OCSPP 835.4200 (anaerobic)][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.####.’ If this review is multilateral, also provide the guideline numbers under which participating agencies are reviewing the study.] |
| Compliance: | [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: | [######] |
| Reviewer: | [Provide final reviewer(s)’s name Signature:and title.] Date: [Type date of signature.] |

**Executive Summary**

The [aerobic or anaerobic] transformation of [type of radiolabel]-labeled [test compound] was studied in [number of] soils for [duration] days in a closed system in darkness at [temperature] °C, pH [value] and [value] soil moisture content at 1/3 bar. The soils were treated at [test concentration] mg a.i./kg, which was equivalent to a field application rate of [value] kg a.i./ha. [Indicate whether anaerobic conditions were maintained in the soil.] Microbial biomass determinations indicated the soils [were or were not] viable at study initiation and termination.

For [soil x], the overall mass balance for the study averaged [value]% of the applied radioactivity (%AR), ranging from [value to value]%AR. For [soil y], the overall mass balance averaged [value]%AR, ranging from [value to value]%AR.

Observed DT50 values, calculated half-lives based on the harmonized NAFTA kinetics guidance (USEPA, 2011), and information on transformation products are listed in Table 1. [Describe whether a reasonable effort was made to maximize recovery of residues. If not, describe whether transformation kinetics calculations were performed for test compound plus unextracted residues as well as for test compound alone.] The amount of extracted radioactivity declined from [value]%AR at study initiation to [value]%AR at day [number]. Unextracted radioactivity increased to [value]%AR at day [number]. The total evolved CO2 and other volatile compounds amounted to [value]%AR and [value]%AR, respectively.

**Table 1. Results Synopsis: [Aerobic or Anaerobic] Soil Metabolism of [Test Compound]**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Compound Name | Observed DT50 (days) | Calculated Half-life (days)Method | Model Parameters and Statistics | **Transformation Products**Common Name (maximum %ARA observed, associated interval) |
| **Major**  | **Minor** |
| [Soil Location][USDA Soil Series][Soil Texture][# °C, pH #] | [value] | [value][method] | [values] | [name] (# %, # days) | [name] (# %, # days) |
| [Soil Location][USDA Soil Series][Soil Texture][# °C, pH #] | [value] | [value][method] | [values] | [name] (# %, # days) | [name] (# %, # days) |
| [Soil Location][USDA Soil Series][Soil Texture][# °C, pH #] | [value] | [value][method] | [values] | [name] (# %, # days) | [name] (# %, # days) |
| [Soil Location][USDA Soil Series][Soil Texture][# °C, pH #] | [value] | [value][method] | [values] | [name] (# %, # days) | [name] (# %, # days) |
| A AR means “applied radioactivity.”[Model parameters include model variables; model statistics include Sc values, correlation coefficients, and p values.] |

[Half-lives and model parameters should be reported for the best fit kinetics model in accordance with the NAFTA kinetics guidance (USEPA, 2011). 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 radiolabel positions.]

**I. Materials and Methods**



**A. Materials:**

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

 Radiochemical purity: [percentage [HPLC or TLC]

 Chemical purity: [percentage (HPLC)]

 Batch number: [value]

 Solubility in water: [value] mg/L at [value] °C

 [If pH-dependent, list available values at each pH and temperature]

**2. Reference Compounds:** The following standards were used in the analysis.

**Table 2. Reference Compounds**

|  |  |  |  |
| --- | --- | --- | --- |
| Applicant’s Code Name | Chemical Name | Purity(%) | Lot No. |
| [code name] | [chemical name] | [#] | [#] |
| [code name] | [chemical name] | [#] | [#] |
| [code name] | [chemical name] | [#] | [#] |
| Data were obtained from [page number] of the study report. [Provide other chemical information in the structure table.] |

**3. Soil:** Soil collection and characterization are summarized in **Table 3** and **Table 4**, respectively. [Characterize any unique properties of soil collection or storage conditions].

Table 3. Description of Soil Collection and Storage

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Description | [Soil Series #1] | [Soil Series #2] | [Soil Series #3] | [Soil Series #4] |
| Geographic location |  |  |  |  |
| Soil series |  |  |  |  |
| Pesticide use history at the collection site |  |  |  |  |
| Collection date |  |  |  |  |
| Collection procedures |  |  |  |  |
| Sampling depth |  |  |  |  |
| Storage temperature |  |  |  |  |
| Storage length |  |  |  |  |
| Soil preparation  |  |  |  |  |
| Data were obtained from page [#] of the study report.  |

Table 4. Properties of the Soils

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Property: | [Soil Series #1] | [Soil Series #2] | [Soil Series #3] | [Soil Series #4] |
| Soil Texture (USDA): |  |  |  |  |
| % Sand  |  |  |  |  |
| % Silt  |  |  |  |  |
| % Clay |  |  |  |  |
| pH (solution)[method] |  |  |  |  |
| Organic carbon (%)[method] |  |  |  |  |
| Organic matter (%)[method] |  |  |  |  |
| Cation Exchange Capacity (meq/100 g)[method] |  |  |  |  |
| CaCO3 equivalence (%) |  |  |  |  |
| Soil Moisture Content (units): |  |  |  |  |
|  At 0.1 bar (pF 2.0) |  |  |  |  |
|  At 1/3 bar (pF 2.5) |  |  |  |  |
| Bulk density(g/cm3) |  |  |  |  |
| Microbial Biomass (units): |  |  |  |  |
|  At initiation |  |  |  |  |
|  During study |  |  |  |  |
|  At termination |  |  |  |  |
| Soil taxonomic classification (USDA or other)[*i.e.*, soil order] |  |  |  |  |
| Data obtained from page [#] of the study report.[The method used to measure pH, organic carbon, organic matter, and CEC should be reported, if available, since the values of these soil properties are method dependent.] |

**B. Study Design:**

1. **Experimental Conditions:** (Summarized in **Table 5**.) [Characterize any unique details of experiential conditions.]

**Table 5. Experimental Design**

|  |  |
| --- | --- |
| Experimental Design | Details |
| Duration of the test (days) |  |
| Soil condition: (Air dried/fresh) |  |
| Soil (g/replicate) |  |
| Application rates: |  |
|  Nominal |  |
|  Actual |  |
| Control conditions (if used)  |  |
| Number of Replicates: |  |
|  Controls ( if used) |  |
|  Treatment |  |
| Test Apparatus: |  |
|  Type/material/volume |  |
|  Details of traps for CO2 and  organic volatiles ( if any) |  |
| If no traps were used, is the system closed/open?  |  |
| Identity and concentration of co-solvent |  |
| Test Material: |  |
|  Volume of the test solution used/treatment |  |
|  Application method  |  |
|  Is the co-solvent evaporated? |  |
| Any indication of the test material adsorbing to the walls of the test apparatus? |  |
| Experimental Conditions: |  |
|  Temperature (°C) |  |
|  Continuous darkness |  |
|  Moisture content |  |
|  Moisture maintenance method |  |
| Other details (if any) |  |
| Data obtained from pages [#] of the study report. |

1. **Sampling During Study Period:** (Details summarized in **Table 6**. Describe any unique characteristics of sampling during study period, if any.)

**Table 6. Sampling During Study Period**

|  |  |
| --- | --- |
| Criteria | Details |
| Sampling intervals (units) |  |
| Sampling method |  |
| Method of collection of CO2 and organic volatile compounds |  |
| Sampling Intervals/Times for:  |  |
|  Sterility check ( if sterile controls are used) |  |
|  Moisture content |  |
|  Redox potential, other |  |
| Sample storage before analysis |  |
| Other observations ( if any) |  |
| Data obtained from pages [#] of the study report. |

1. **Analytical Procedures:**

Extraction Methods: [Briefly describe the extraction method. An example follows. Be sure to describe the effectiveness of the soil extraction process. Solvent selection should be sufficiently robust to ensure extraction of bound residues.]

Soil samples were extracted [# of extractions] with [solvent system] (%:%, v:v) by [extraction method] for [#] minutes per extraction ([report page reference]). After each extraction, the mixtures were centrifuged and the supernatant decanted. Extracts were combined, diluted with [solvent], and pH adjusted [pH value] using [dilution solvent]. Aliquots of the combined extracts were analyzed for total radioactivity using [analytical method].

Aliquots of the combined extracts were concentrated under a stream of [gas] in a waterbath, diluted with [dilution solvent] and filtered (# μm). Aliquots of the concentrated solutions were analyzed by [analytical method].

Determination of Unextracted Residues:

Portions ([# x *#* g]) of the extracted soils were air-dried, ground with a mortar and pestle, then analyzed for total radioactivity by [analytical method] followed by combustion ([report page reference]). In addition, portions of the [termination day] extracted soils were further analyzed to determine the concentrations of fulvic acid, humic acid, and humin ([report page reference]). The extracted soils were extracted with [extraction solvent], then centrifuged. The soil pellet was combusted to quantify the soil humin fraction. The supernatant was adjusted to pH [value] then centrifuged. The resulting supernatant (fulvic acid) and precipitate (humic acid) were analyzed using [analytical method].

Determination of Volatile Compounds:

Aliquots ([# x # mL]) of the volatile trapping solutions were analyzed for total radioactivity using [analytical method] ([report page reference]). The presence of CO2 in the KOH trapping solution was confirmed by precipitation with saturated barium chloride ([report page reference]).

Total Radioactivity Measurement:

Total 14C residues were determined by summing the concentrations of residues measured in the soil extracts, extracted soil and volatile trapping solutions ([report page number]).

Derivatization Method: [Describe derivatization method, if employed.].

Identification and Quantification of Parent Compound:

Aliquots of the soil extracts were analyzed using [analytical method (i.e., HPLC)] under the following conditions: [describe instrument, column, mobile phase, gradient, and UV (# nm) and radiochemical detection ([report page number]). Radiolabeled [parent compound] was identified by comparison to the retention time of an unlabeled reference standard (purity [%], retention time (Rt) ([# to #] minutes) that was co-chromatographed with the samples ([report page number]). Column recovery determined prior to analysis of the definitive samples was [#] % ([report page number]). In addition, the identification of [parent compound] was confirmed by [analytical method (*i.e.*, LC-MS/MS)] with electrospray ionization in the positive mode ([report page number]).

Detection Limits (LOD, LOQ) for the Parent Compound:

The limit of detection (LOD) was determined to be [percentage] of the applied radioactivity (%AR), with a limit of quantitation (LOQ) at [percentage] AR.

Detection Limits (LOD, LOQ) for the Transformation Products:

The LOD and LOQ were the same as parent ([report page number]).

II. Results and Discussion

1. **Data:**

Study results including total mass balances and distribution of radioactivity are presented in **Table 7**. [Indicate the results of any checks on aerobic or anaerobic conditions and viability of test soils. If applicable, report redox conditions.]

1. **Mass Balance:**

The mass balance and distribution of radioactivity from each soil are shown in **Table 7**. Recoveries ranged from [percentage] to [percentage] of the applied radioactivity (%AR). Unidentified residues accounted for [percentage]AR. [If there is a large amount of unidentified radioactivity, mention it here. Indicate whether there was substantial loss of radioactivity by sorption to glassware or volatilization. Also mention if the mass balance meets guideline criteria.]

1. **Bound and Extractable Residues:**

The amount of extractable radioactivity declined from [percentage]AR at time zero to [percentage]AR at day [number] for [test compound]. Unextracted radioactivity increased to [percentage]AR at day [number]. [If unextracted residues were >10% of the applied, discuss whether the sediment extraction procedures were reasonable and whether the unextracted residues may include available residues.]

1. **Volatilization:**

Volatiles [were/were not] trapped. Volatile radioactivity, identified as evolved 14CO2 represented [percentage]AR at day [number] for [test compound]. [Add information regarding additional volatile chemicals as needed.]

|  |
| --- |
| **Table 7. Transformation of [test compound], Expressed as a Percentage of Applied Radioactivity in [Soil Series]** |
| **Sampling Interval (days)** | Interval # | Interval # | Interval # | Interval # | Interval # | Interval # | Interval # | Interval # | Interval # | Interval # | Interval # |
| **Replicate Number** | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 |
| [Parent compound] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| [Transformation product #1] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| [Transformation product #2] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| [Others] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| Extracted residues | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| Unextracted residues | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| CO2 | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| Volatile organics | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |
| Mass balance | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] | [#] |

[Repeat this table as needed for additional soils. Note that individual replicate values are tabulated rather than means and standard deviations.]

1. **Transformation of Test Compound:**

Degradation of [radiolabel-test compound] on soil was [gradual, rapid, or some other characterization]. The calculated half-life ranged from [x] to [x] days, as tabulated in **Table 8** (calculated half-lives and model parameters for the best fit kinetics models are in bold). [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. Discuss any abnormalities observed in the data.]

[Images of kinetics calculation results using the R program may replace **Table 8**. R images should include the model parameters and statistics that are otherwise reported in **Table 8**.]

**Table 8. Transformation Kinetics of [Test Compound] in Soil A, B**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Observed DT50 (days) | Observed DT90 (days) | CalculatedHalf-life(days) | Kinetics Model C | Model Parameters | Model Statistics |
| [Soil Location][USDA Soil Series][Soil Texture][# °C, pH #] | [#] | [#] | [#] | SFO | C0=[#], k=[#] | SSFO=[#], r2=[#], p=[#] |
| [#] | IORE | C0=[#], k=[#], n=[#] | SIORE=[#], SC=[#], r2=[#], p=[#] |
| [#] | DFOP [if applicable] | C0=[#], g=[#], k1=[#], k2=[#],  | SDFOP=[#], r2=[#], p=[#] |
| [Soil Location][USDA Soil Series][Soil Texture][# °C, pH #] | [#] | [#] | [#] | SFO | C0=[#], k=[#] | SSFO=[#], r2=[#], p=[#] |
| [#] | IORE | C0=[#], k=[#], n=[#] | SIORE=[#], SC=[#], r2=[#], p=[#] |
| [#] | DFOP [if applicable] | C0=[#], g=[#], k1=[#], k2=[#],  | SDFOP=[#], 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 Calculated half-lives and model parameters for the best fit kinetics models, in accordance with the NAFTA kinetics guidance (USEPA, 2011), are in bold.C Kinetics models: Single First-Order (SFO); Double First-Order in Parallel (DFOP), and Indeterminate Order Rate Equation (IORE). |

[Rows may be added for transformation product half-lives and DT50s as needed. Half-lives should be calculated following the NAFTA kinetics guidance (USEPA, 2011). 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 radiolabel positions.]

[Briefly summarize the transformation products per system in Table 9. If transformation product decline is observed over four time intervals, calculate a half-life and discuss the pattern of decline.]

**Table 9. Transformation Products of [Test Compound] in Soil**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Transformation Product(s) | Maximum %AR Observed | Associated Interval | Final %AR Observed | Final Interval |
| [Soil Location][USDA Soil Series][Soil Texture][# °C, pH #] | [common name] | [#] | [# d] | [#] | [# d] |
| [common name] | [#] | [# d] | [#] | [# d] |
| [Soil Location][USDA Soil Series][Soil Texture][# °C, pH #] | [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. Aerobic/Anaerobic Soil Degradation Pathway of [radiolabel-test compound]]**

**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[[1]](#footnote-1). 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.]

[The attached Excel file has three example spreadsheets for pe + pH (for anaerobic studies), mass balance, and kinetics calculations.]

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 9.

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

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

Indeterminate Order Rate Equation (IORE) Model

$C\_{t}=\left[C\_{0}^{\left(1-N\right)}-\left(1-N\right)k\_{IORE}t\right]^{\left(\frac{1}{1-N}\right)}$ (eq. 4)

where,

 N = order of decline rate (-)

 kIORE = IORE rate constant of decline (d-1)

This equation is solved [with the Excel Solver] by adjusting *C0*, *kIORE*, and *N* to minimize the objective function for IORE (SIORE) (See equation 9). Half-lives for the IORE model are calculated using equation 5, which represents a first-order half-life that passes through the DT90 of the IORE model. (Traditional DT50 and DT90 values for the IORE model can be calculated using equations 6 and 7.)

$t\_{IORE}=\frac{log⁡(2)}{log(10)}\frac{C\_{0}^{1-N}\left(1-0.1^{(1-N)}\right)}{\left(1-N\right)k\_{IORE}}$ (eq. 5)

DT50 =  (eq. 6)

DT90 =  (eq. 7)

Double First-Order in Parallel (DFOP) Model

$C\_{t}=C\_{0}g^{-k\_{1}t}+C\_{0}\left(1-g\right)^{-k\_{2}t}$ (eq. 8)

where,

 g = the fraction of C0 applied to compartment 1 (-)

 k1 = rate constant for compartment 1 (d-1)

 k2 = rate constant for compartment 2 (d-1)

If *C0 x g* is set equal to *a* and *C0(1-g)* is set equal to *c*, then the equation can be solved [with the Excel Solver] for *a*, *c*, *k1*, and *k2* by minimizing the objective function (SDFOP) as described in equation 9.

DT50 and DT90 values can be calculated using equations 2 and 3, with k1 or k2 in place of k.

Objective Function: SFO, IORE, and DFOP are solved by minimizing the objective function (SSFO, SIORE, or SDFOP).

$S\_{SFO},S\_{IORE},or S\_{DFOP}=\sum\_{}^{}(C\_{model},t-C\_{d,t})^{2}$ (eq. 9)

where,

SSFO , SIORE, or SDFOP = objective function of kinetics 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 (%)

Critical Value to Determine Whether SFO is an Adequate Kinetics Model

If SSFO is less than SC, the SFO model is adequate to describe kinetics. If not, the faster of tIORE or the DFOP DT50 for compartment 2 should be used.

$S\_{c}=S\_{IORE}\left(1+\frac{p}{n-p}F\left(α,p,n-p\right)\right)$ (eq. 10)

where,

Sc = the critical value that defines the confidence contours (%2)

p = number of parameters (3 in this case)

α = the confidence level (0.50 in this case)

F(α, p, n-p) = F distribution with αlevel of confidence and degrees of freedom p and n-p

1. 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-1)