SERA TR-056-13-01-02b

Chlorothalonil:
WorksheetMaker Workbook Documentation
FINAL REPORT

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(August 27, 2015 minor corrections)

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LIST OF INPUT FILES

Chlorothalonil WMS Formulation Inputs.docx
Chlorothalonil WSM Chemical Inputs.docx

Note that the input files are for the SERA 2011b utility. These are customized based on current information for the JH Stone Nursery.

Revision Note

Initial

This is a modification to SERA TR-056-13-01-01c, Chlorothalonil: WorksheetMaker Workbook Documentation, dated December 8, 2014. Changes to this report are based on the following comments from the Forest Service:

- Notes from John Justin and Shawna Bautista in an EXCEL workbook (**Daconil Action Backpack Directed Foliar-SB.xlsm**) via an email from Shawna Bautista dated 6/2/2015.
- Comments from John Justin in a Microsoft Word file (**Query Template for WSM Input Effort.docx**) via an email from Shawna Bautista dated 12/30/2014.
- Review comments from Shawna Bautista embedded in a copy of SERA TR-056-13-01-01c and transmitted as a Microsoft Word file (**Chlorothalonil WSM Documentation SERA TR-056-13-01-01c-SB.docx**).

The most recent set of comments (i.e., the EXCEL workbook from 6/2/2015) is given precedence when the feedback is inconsistent.

August 27, 2015

The statement at the top of Page 4 (Lines 4-5) concerning the use of respirators has been clarified.

ACRONYMS, ABBREVIATIONS, AND SYMBOLS

ACGIH	American Conference of Governmental Industrial Hygienists
ADI	Acceptable Daily Intake
AEL	adverse-effect level
a.e.	acid equivalent
a.i.	active ingredient
a.k.a.	also known as
a.s.	active substance
AOEL	acceptable occupational exposure limit
APHIS	Animal and Plant Health Inspection Service
ATSDR	Agency for Toxic Substances and Disease Registry
ASAE	American Society of Agricultural Engineers
BCF	bioconcentration factor
bw	body weight
calc	calculated value
CBI	confidential business information
CI	confidence interval
cm	centimeter
CNS	central nervous system
COC	crop oil concentrates
DAA	days after application
DAT	days after treatment
DER	data evaluation record
d.f.	degrees of freedom
EC	emulsifiable concentrate
EC_x	concentration causing X% inhibition of a process
EC_{25}	concentration causing 25% inhibition of a process
EC_{50}	concentration causing 50% inhibition of a process
ECOTOX	ECOTOXicology (database used by U.S. EPA/OPP)
EFED	Environmental Fate and Effects Division (U.S. EPA/OPP)
ERA	ecological risk assessment
ExToxNet	Extension Toxicology Network
F	female
FH	Forest Health
FIFRA	Federal Insecticide, Fungicide and Rodenticide Act
FQPA	Food Quality Protection Act
g	gram
GLP	Good Laboratory Practices
ha	hectare
HEC	human equivalent concentration
HED	Health Effects Division (U.S. EPA/OPP)
HHRA	human health risk assessment
HIARC	Hazard Identification and Assessment Review Committee (part of U.S. EPA/OPP/HED)
HQ	hazard quotient
HRAC	Herbicide Resistance Action Committee
IARC	International Agency for Research on Cancer

IC_{50}	concentration causing 50% inhibition
IRED	Interim Reregistration Eligibility Decision
IRIS	Integrated Risk Information System
k_a	absorption coefficient
k_e	elimination coefficient
kg	kilogram
$K_{o/c}$	organic carbon partition coefficient
$K_{o/w}$	octanol-water partition coefficient
K_p	skin permeability coefficient
L	liter
lb	pound
LC_{50}	lethal concentration, 50% kill
LD_{50}	lethal dose, 50% kill
LOAEL	lowest-observed-adverse-effect level
LOC	level of concern
LR_{50}	50% lethal response [EFSA/European term]
m	meter
M	male
mg	milligram
mg/kg/day	milligrams of agent per kilogram of body weight per day
mL	milliliter
mM	millimole
mPa	millipascal, (0.001 Pa)
MOS	margin of safety
MRID	Master Record Identification Number
MW	molecular weight
NOAEL	no-observed-adverse-effect level
NOEC	no-observed-effect concentration
NOEL	no-observed-effect level
NOS	not otherwise specified
N.R.	not reported
OPP	Office of Pesticide Programs
ppm	parts per million
RED	re-registration eligibility decision
RfD	reference dose
SDS-3701	4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene
SERA	Syracuse Environmental Research Associates
T.G.I.A.	Technical grade active ingredient
UF	uncertainty factor
U.S.	United States
USDA	U.S. Department of Agriculture
U.S. EPA	U.S. Environmental Protection Agency
USGS	U.S. Geological Survey
WHO	World Health Organization

1. INTRODUCTION

1.1. General Information

This document supports the development of a WorksheetMaker EXCEL workbook for the subject pesticides. As detailed in SERA (2011a), WorksheetMaker is a utility that automates the generation of EXCEL workbooks that accompany Forest Service risk assessments, and these EXCEL workbooks are typically generated in the development of Forest Service risk assessments (SERA 2014).

The development of full Forest Service risk assessments, however, is resource intensive. For some pesticides that are used in only relatively small amounts and/or only in few locations, the development of full Forest Service risk assessments is not feasible. Nonetheless, the Forest Service may be required to develop risk analyses supported by WorksheetMaker EXCEL workbooks. To meet this need, an MS Word utility was developed to facilitate the addition of pesticides and pesticide formulations into the Microsoft Access database used by WorksheetMaker (SERA 2011b). With this addition, WorksheetMaker can be used to generate EXCEL workbooks typical of those that accompany Forest Service risk assessments.

The current document is designed to serve as documentation for the application of this general method for the pesticide discussed in Section 1.2. The major difference between this approach to using WorksheetMaker and the typical use of WorksheetMaker in the development of Forest Service risk assessments involves the level of documentation and the sources used in developing the documentation. While standard Forest Service risk assessments involve a relatively detailed review and evaluation of the open literature and publically available documents from the U.S. EPA, as discussed further in Section 1.2, the current assessment relies primarily on secondary sources with minimal independent evaluation of the data.

While this document and the accompanying EXCEL workbook are intended to be generically useful within the Forest Service, the program/project specific inputs are based on uses at the JH Stone nursery in Central Point, Oregon, with information provided by John Justin (Nursery Manager) and Shawna Bautista (Forest Service Pesticide Use Coordinator). While these program/project specific inputs are used in the current report, all rates, volumes, acres treated, number of applications, and other estimates are estimated based on annual averages. Actual inputs used in a specific application at the JH Stone nursery are determined based on the degree of pest infestation and the acres of the crop to be treated. In assessing an actual application at the JH Stone nursery or other facility or forest, this report and the accompanying WorksheetMaker workbook should be modified using inputs relevant to the specific application.

1.2. Chemical Specific Information

The current document concerns chlorothalonil. Most of the information on chlorothalonil was identified at the U.S. EPA's Pesticide Chemical Search website (http://iaspub.epa.gov/apex/pesticides/f?p=CHEMICALSEARCH:1:11098277289067::NO:1::) using the search term "chlorothalonil." Chlorothalonil is a fungicide. U.S. EPA's Pesticide Chemical Search website lists 5 regulatory action documents on chlorothalonil, 521 cleared science reviews, and 2 E-Dockets (EPA-HQ-OPP-2011-0840 and EPA-HQ-OPP-2010-0014). TOXLINE (http://toxnet.nlm.nih.gov) contains 4827 open literature citations using synonyms and 1241 not using synonyms. The distinction between using and not using synonyms is

important in that using synonyms may lead to irrelevant citations (most often due to formulation names) and not using synonyms may result in missing some relevant citations. The review of the open literature relating to ecotoxicology by U.S. EPA/OPP/EFED (2012, Appendix H) contains a 212-page list of more than 2500 open literature publications, 119 of which are classified as 'acceptable' to OPP. Based on this cursory examination, the open literature on chlorothalonil may be characterized as extensive.

For the current documentation, information on human health effects is taken primarily from the human health risk assessment scoping document for the registration review of chlorothalonil (U.S. EPA/OPP/HED 2012) supplemented by information in the RED for chlorothalonil (U.S. EPA/OPP 1999a) and a more recent review by the California Department of Pesticide Regulation (CalDPR 2005). Information on ecological effects and the environmental fate of chlorothalonil is taken primarily from the EPA's assessment of the potential effects of chlorothalonil on threatened and endangered species (U.S. EPA/OPP/EFED 2012) with supplemental information from Tomlin (2004) and ChemIDplus (2014).

This document is accompanied by two MS Word files: **Chlorothalonil WMS Formulation Inputs.docx** and **Chlorothalonil WSM Chemical Inputs.docx**. These files can be used with the MS Word utility, SERA (2011b), to add chlorothalonil to the database used by WorksheetMaker. This document is also accompanied by a WorksheetMaker EXCEL workbook, **Chlorothalonil SAMPLE Workbook.xlsm**. Forest Service personnel may then modify this workbook for program specific activities.

2. CHEMICAL/PHYSICAL PROPERTIES

Chlorothalonil has been used in the United States since 1966 on turfgrass and since 1970 on crops. Chlorothalonil is a fungicide used primarily to control fungal foliar diseases on vegetables, other field crops, and ornamentals (U.S. EPA/OPP 1999a). Chlorothalonil was originally developed by Diamond Alkali Co. and later sold to Syngenta (Tomlin 2004).

The U.S. EPA registration review program operates on a 15-year cycle. Chlorothalonil is currently under registration review (U.S. EPA/OPP 2012). A final work plan detailing the schedule for the complete registration review process has not been identified.

The PAN Pesticides Database currently lists 327 active formulations of chlorothalonil (Kegley et al. 2014). The U.S. EPA/OPP (1999b) indicates that 101 formulations with 98 Special Local Needs registrations are available. As of 2011 (the most recent year for which data are available), the USGS estimates that about 10 million pounds of chlorothalonil are used annually in agricultural applications (http://water.usgs.gov/nawqa/pnsp/usage/maps/show_map.php?year=2011&map=CHLOROTHALONIL&hilo=L&disp=Chlorothalonil). Based on the most recent EPA risk assessment (i.e., U.S. EPA/OPP/EFED 2012, Table 2-5), the maximum single application rates for chlorothalonil range from less than to 11 lb a.i./acre, and the maximum cumulative annual application ranges from less than 1 to up to 26 lb a.i./acre.

Based on Forest Service comments on the original WMS workbook, the application rate will be 2.1 lbs a.i./acre with an application volume of 30 gallons/acre. Five acres may be treated in a single application lasting 1 hour. Up to 30 acres may be treated annually. Thus, it appears that six different 5-acre sites may be treated over the course of 1 year.

Application methods may include broadcast spray through tractor mounted spray booms or directed foliar backpack spray. Based on comments from the Forest Service on the original WorksheetMaker workbook, the current report and the accompanying workbook are based on ground broadcast applications—i.e., a tractor calibrated to 30 gallons/acre. A single worker may handle up to 6.3 lbs a.i./day. Note that this is equivalent to a single worker treating 3 acres at an application rate of 2.1 lbs a.i./acre. Worker PPE will include chemical resistant gloves made of any water resistant material, protective eyewear, shoes plus socks, chemical resistant apron when mixing or loading.

The WorksheetMaker workbook that accompanies this risk assessment is based on an October 7, 2008 label for Daconil WeatherStick obtained from Syngenta web site (http://www.syngentacropprotection.com/pdf/labels/daconilweastik0100.pdf). The label is designated as ZPP-DAC-027 01/00. As specified by the Forest Service, this formulation contains 54% a.i. The product label specifies that this is equivalent to 6 lbs a.i./gallon (720 g a.i./L). The product label for Daconil WeatherStick notes the following:

> *For exposures in enclosed areas, applicators and other handlers must wear a respirator with either an organ vapor-removing cartridge with a prefilter approved for pesticides (MSHA/NIOSH approval number prefix TC-23C), or a canister approved for pesticides (MSHA/NIOSH approval number prefix TC-*

14G), or a NIOSH approved respirator with an organic vapor (OV) cartridge or canister with any N,R, P, or HE prefilter.

Note that the Forest Service has not indicated that a respirator will be used, presumably because chlorothalonil will not be applied in enclosed areas.

Based on information from the Forest Service (the illustration in **JH Stone Nursery Information-v3 Shawna Aug 21.docx**), the JH Stone nursery is about 220 acres in size. Using a 30-acre treated area, a proportion of about 0.14 [30 acres ÷ 220 acres ≈ 0.136363] of the nursery area would be treated. As discussed further in Section 3.2.2.1, this proportion is used to modify the water contamination rates.

Table 1 summarizes the chemical and physical properties of chlorothalonil. As reviewed by U.S. EPA/OPP/EFED (2012), aqueous photolysis appears to be the primary route of degradation for chlorothalonil with a half-life of about 0.4 days. Microbial degradation appears to be kinetically complex and not well characterized by first-order kinetics. In the current analysis (as well as U.S. EPA/OPP/EFED 2012), environmental fate modeling is based on first-order kinetics. Chlorothalonil does not appear to be highly persistent in either soil (aerobic half-lives of 0.3 to 58 days) or water (aerobic half-lives of 0.05 to 3.4 day; anaerobic half-times of 4.8 to 10.6 days). Chlorothalonil is somewhat lipophilic (with a K_{ow} of about 1000) and will bind moderately to soil (K_{oc} ranges from about 1000 to 11,000), and can bioconcentrate in fish (whole fish BCFs of about 3000).

As discussed in U.S. EPA/OPP/EFED (2012, Section 1.2.2), chlorothalonil is extensively metabolized in the environment, and one metabolite of concern has been identified—i.e., 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene or SDS-3701. As discussed further in Section 4, this metabolite is more toxic than chlorothalonil to mammals and birds but is less toxic than chlorothalonil to aquatic organisms.

3. HUMAN HEALTH

3.1. Hazard Identification

As summarized in Table 1, the fungicidal activity of chlorothalonil is associated with an inhibition of glycolysis (Tomlin 2004; CalEPA 2006)—i.e., the anaerobic metabolism of glucose to pyruvate; however, the precise mechanism of action in fungi is unclear (U.S. EPA/OPP/EFED 2012). In mammals, the mechanism of action appears to involve the generation of cysteine S-conjugates of chlorothalonil that are toxic to the kidney (U.S. EPA/OPP/HED 2012, p. 7).

The U.S. EPA/OPP/HED (2012) classifies chlorothalonil as highly toxic (Category I) on inhalation (acute LC_{50} of 0.02 mg/L) and ocular exposure, relatively non-toxic on oral or dermal exposure (Category IV), and moderately toxic for dermal irritation (Category III). In addition, chlorothalonil is not classified as a skin sensitizer.

As discussed further in Section 3.3, toxicity to the kidney is the most sensitive endpoint in mammals and is the basis for the development of RfDs. As part of the registration review, the EPA is requiring a 90-day inhalation toxicity study, an immunotoxicity study, and an acute

neurotoxicity study (U.S. EPA/OPP/HED 2012, p. 6). In addition, the EPA is requiring screening tests of chlorothalonil for endocrine disruption (U.S. EPA/OPP/HED 2012, p. 10). Once these studies are completed, the EPA may reevaluate the dose-response assessment for chlorothalonil.

Chlorothalonil is classified as "likely" to be a human carcinogen (U.S. EPA/OPP/HED 2012, p. 29). This classification appears to be based on the development of forestomach tumors in rodents. In the absence of data indicating that chlorothalonil is carcinogenic, the EPA does not use a linear non-threshold model to calculate excess lifetime risks of cancer (U.S. EPA/OPP/HED 2012, p. 3).

The U.S. EPA/OPP/HED (2012, p. 12) identifies the 4-hydroxy metabolite of chlorothalonil as a metabolite of concern.

3.2. Exposure Assessment

3.2.1. Workers

3.2.1.1. General Exposures

As discussed in SERA (2014b), the Forest Service risk assessments use a standard set of worker exposure rates (Table 14 in SERA 2014b).

As noted in Section 3.1, the U.S. EPA/OPP/HED (2012) classifies chlorothalonil as Category IV (the least toxic category) for dermal toxicity. Consequently, dermal risk is not quantified since no hazard was identified via the dermal route for chlorothalonil (U.S. EPA/OPP/HED 2012, p. 14). In the early Reregistration Eligibility document (RED), U.S. EPA/OPP (1999a, p. 23) uses an upper limit of 0.15% dermal absorption for a workday. This dermal absorption rate is estimated from the ratio of dermal to oral LOAELs from subchronic toxicity studies. This dermal absorption rate corresponds to an estimated first-order dermal absorption rate of about 0.00019 $hour^{-1}$ [k_a = -ln(1-0.0015)÷8 hours ≈ 0.0001976 $hour^{-1}$]. The EPA does not provide an estimate of the variability in the k_a. As noted by Feldman and Maibach (1974, p. 131) in their article on the dermal absorption of pesticides, *…1 person in 10 will absorb twice the mean value while 1 in 20 will absorb 3 times this amount*. Based on this observation, the central estimate of the k_a is divided by a factor of 3 to approximate a 95% lower bound and multiplied by a factor of 3 to approximate a 95% upper bound. Thus, the dermal absorption rates used for chlorothalonil in this analysis are 0.00019 $hour^{-1}$ (0.000063 to 0.00057) $hour^{-1}$.

In the absence of experimental data, Forest Service risk assessments use an algorithm based on the molecular weight and octanol water partition coefficient (K_{ow}) to approximate a first-order dermal absorption rate coefficient (see Eq. 23, Section 3.1.3.2.2 in SERA 2014a). As detailed in Worksheet B03b of the WorksheetMaker workbook that accompanies this report, the estimated first-order dermal absorption rate coefficient based on this algorithm is 0.0077 (0.0030 to 0.0196) $hour^{-1}$ based on a molecular weight of 269.9 and K_{ow} of 6309 (Table 1 values from EPA/OPP/EFED 2012, Table 3-1). The central estimate of 0.0077 $hour^{-1}$ is higher than the EPA estimate by a factor of about 40 [0.0077 $hour^{-1}$ ÷ 0.00019 $hour^{-1}$ ≈ 40.526]. Nonetheless, the current document defers to the more detailed analysis from U.S. EPA/OPP (1999a).

As discussed in Section 2, the WorksheetMaker workbook that accompanies this risk assessment is based on ground broadcast applications. As detailed in Table 14 of SERA (2014b), the reference chemical for this application method is 2,4-D with a first-order dermal absorption rate of 0.00066 $hour^{-1}$. The central estimate of the dermal absorption rates used for chlorothalonil in this analysis are 0.00019 $hour^{-1}$. The central estimate of the worker exposure rate for ground broadcast applications of 2,4-D 0.0001 with a 95% prediction interval of 0.000002 to 0.005 mg/kg bw per lb a.i. handled. To account for differences in the estimated dermal absorption of chlorothalonil and 2,4-D, the worker exposure rates for 2,4-D are multiplied by the ratio of the dermal absorption rate coefficient for chlorothalonil to the corresponding value for 2,4-D ($0.00019 \div 0.00066 \approx 0.287$). These calculations are detailed in Table 2. Following the convention in SERA (2014b), the resulting worker exposure rates are rounded to one significant digit, and the occupational exposure rates for ground broadcast applications of chlorothalonil are estimated as 0.00003 (0.0000006 to 0.001) mg/kg bw per lb handled.

Another important factor in worker exposures is the amount of pesticide that a worker will handle. As indicated in Worksheet C01 of the workbook that accompanies this report, the amount that a worker would handle is estimated at 10.5 lbs based on the treatment of 5 acres at an application rate of 2.1 lb a.i./acre. As discussed in Section 2, these amounts are based on inputs from the Forest Service for the JH Stone Nursery.

3.2.1.2. Accidental Exposures

In addition to general exposures, four standard accidental exposure scenarios for workers discussed in SERA (2014a, Section 3.2.2.2) are also considered, the details of which are provided in Worksheets C02a,b and C03a,b.

Worksheets C03a,b involve accidental spills under the assumption of first-order dermal absorption. These scenarios use the same first-order dermal absorption rate coefficients discussed in Section 3.2.1.1.

Worksheets C02a,b involve contaminated gloves under the assumption of zero-order dermal absorption. These scenarios require an estimate of the skin permeability coefficient (K_p in units of cm/hr). No experimental measurements of K_p were identified in the literature reviewed for this report (Section 1.2). Consequently, the K_p is estimated using an algorithm developed by the U.S. EPA's Office of Research and Development as discussed in SERA (2014a, 3.1.3.2.1). The application of this algorithm to chlorothalonil is detailed in Worksheet B03a of the WorksheetMaker workbook that accompanies this document. These values are rounded to 0.027 (0.013 to 0.060) cm/hr in Worksheets C02a,b.

3.2.1.3. Inhalation Exposures

As noted in Section 3.1, chlorothalonil is classified by the EPA as highly toxic (Category I) via inhalation. U.S. EPA/OPP/HED (2012) uses monitoring data rather than modeling to assess inhalation exposures in workers. As summarized in Table 3 of the current document, monitoring studies report peak concentrations of 23 to 737 ng/m^3 and mean concentrations of 17 to 262 ng/m^3 at application sites. A major limitation of these monitoring data is that the concentrations are not explicitly associated with defined application rates. Consequently, these data are not incorporated into the WorksheetMaker workbook that accompanies this document.

Recognizing limitations in the currently available data, U.S. EPA/OPP/HED (2014) indicates that additional applicator exposure monitoring is being required. The Agency also notes that revisions to the worker risk assessment may be made as the registration review continues.

> *As more-reliable data become available …, the Agency will continue to replace existing exposure data. As a result, occupational handler scenarios may need to be revisited during Registration Review.*
>
> U.S. EPA/OPP/HED 2014, p. 17.

Consistent with the approach taken in U.S. EPA/OPP/HED (2012), the current document characterizes risks to workers based on the currently available monitoring data (Section 3.4.1). As noted by U.S. EPA/OPP/HED (2014, p. 16), these data are also applicable to bystander exposures.

A more refined analysis, involving the use of the Industrial Source Complex Short Term model (U.S. EPA/OAQPS 1995) model, could be considered but is beyond the scope of the current document. In addition, further and more detailed analyses could be of questionable use, depending on the final assessment of inhalation exposures to chlorothalonil in the registration review.

Exposure assessments based on monitoring data could overestimate exposures if respiratory personal protective equipment (PPE) is used. As discussed in Section 2, the Forest Service has not indicated that respiratory PPE will be used, and respiratory PPE is not required unless chlorothalonil is applied in enclosed spaces.

3.2.2. General Public

As detailed in SERA (2014a, Section 3.2.3), Forest Service risk assessments provide a standard set of exposure scenarios for members of the general public. These exposure scenarios are applicable to standard forestry applications of pesticides and are not included in the WorksheetMaker workbook that accompanies this document. Sections 3.2.2.1 through 3.2.2.4 below, however, discuss chemical specific inputs that are used in the workbook.

3.2.2.1. Surface Water

While most of the exposure scenarios given in the WorksheetMaker workbook are standard for Forest Service risk assessments, one notable exception is the surface water modelling. Full Forest Service risk assessments typically estimate concentrations of a pesticide in surface water using GLEAMS-Driver (SERA 2014a, Section 3.2.3.4.3). In the interest of economy, the current analysis uses FIRST (FQPA Index Reservoir Screening Tool). FIRST is a Tier 1 model developed by the U.S. EPA to estimate concentrations of pesticide in surface water, and details of the FIRST model are available at http://www.epa.gov/oppefed1/models/water/first_description.htm.

The input parameters and the estimated concentrations of chlorothalonil in surface water are summarized in Table 4. The output files from the simulations in FIRST are given in Appendix 1. As with standard GLEAMS-Driver modeling, a unit application rate of 1 lb a.i./acre is used. The results from the modeling are entered into Worksheet B04Rt as water contamination rates—i.e., mg/L per lb a.i./acre applied.

One very important input parameter for FIRST is the proportion of the watershed that is treated. As indicated in Table 4, the FIRST modeling was conducted using a proportion of 1.0—i.e., the entire watershed is treated. In some applications, the concentrations given in Table 4 could be adjusted downward if only a fraction of the area under consideration (i.e., the relevant watershed) is treated.

The current analysis is focused on the JH Stone Nursery. As discussed in Section 2, the current analysis anticipates that about 0.14 of the nursery's fields would be treated with chlorothalonil. As also illustrated in Table 4, this proportion is used to reduce the surface water concentrations anticipated at the JH Stone nursery. Since the watershed in the vicinity of the JH Stone nursery is larger than the area of the nursery itself, this approach is conservative in that the concentrations of chlorothalonil in surface water are probably grossly over-estimated.

3.2.2.2. Vegetation

As detailed in SERA (2014a, Section 3.2.3.7), several scenarios involving the consumption of contaminated vegetation are included in workbooks produced by WorksheetMaker for pesticides applied to foliage. The major input parameters are application rate, number of applications, and application interval.

For longer-term exposures, half-lives on vegetation are also important parameters. Very little information is available in the literature reviewed (Section 1.2) on the kinetics of chlorothalonil on vegetation. As summarized in Table 1, Knisel and Davis (2000) report a foliar half-life of 10 days, and U.S. EPA/OPP/EFED (2012) uses a default half-life of 35 days, based on the extensive review by Willis and McDowell (1987). For the current assessment, the half-lives on vegetation (foliage) are taken as 20 (10 to 35) days with the central estimate based on the approximate geometric mean of the half-lives of 10 days and 35 days.

As also summarized in Table 1, the review by Willis and McDowell (1987, Table VI, p. 55) reports a half-life of 4.1 ± 1.5 days on apples. Based on this report, the half-lives on fruit are taken as 4.1 (2.6 to 5.6) days. Note that Willis and McDowell (1987) do not explicitly characterize the "±" as a range or standard deviation.

3.2.2.3. Bioconcentration

As discussed in SERA (2014a, Section 3.2.3.5), scenarios involving the consumption of contaminated vegetation are included in most WorksheetMaker workbooks. The major chemical specific inputs are the concentrations in surface water (discussed in Section 3.2.1.1 of this document) and the bioconcentration factor (BCF). For exposure scenarios involving humans, the BCF is based on the edible portion (muscle) in fish. For the ecological risk assessment, the BCF is based on whole fish. When adequate data are available, separate BCF values may be given for acute exposures and longer-term exposures.

As summarized in Table 1, U.S. EPA/OPP/EFED (2012) reports bioconcentration factors for chlorothalonil at two concentrations (0.1 and 0.5 µg/L) for the edible portion of fish and whole fish. While the differences in the bioconcentration factors are not substantial, the BCFs for the higher concentrations are used for acute exposure scenarios and the BCFs for the lower concentrations are used for longer-term exposure scenarios.

Based on the BCF values for the edible portion on fish in Table 1, a BCF 306 is used for acute exposure scenarios and a BCF of 256 is used for longer term exposure scenarios.

3.2.2.4. Dermal Exposure

As in the accidental exposure assessments for workers (Section 3.2.1.2 of the current document), dermal exposure scenarios involving both first-order and zero-order absorption are used in scenarios for members of the general public. Details of these exposure scenarios are given in SERA (2014a—i.e., Section 3.2.3.3 for contaminated vegetation and Section 3.2.3.6 for swimming. The dermal absorption values used in these scenarios are identical to those used for workers.

3.3. Dose-Response Assessment

The dose-response assessments for chlorothalonil are summarized in Table 5. All toxicity values are taken from the most recent EPA human health risk assessment (U.S. EPA/OPP/HED 2012).

Chlorothalonil is somewhat atypical in that the U.S. EPA/OPP/HED derived both oral and inhalation toxicity values (U.S. EPA/OPP/HED 2012). The oral toxicity values are incorporated into the WorksheetMaker workbook that accompanies this document. As discussed in Section 3.2.1.3, the exposure data used in the risk characterization (Section 3.4.1) are based on monitoring data not explicitly associated with an application rate. Consequently, the inhalation toxicity data are not used in the WorksheetMaker workbook.

3.3.1. Oral Toxicity

The two oral toxicity values are used in the WorksheetMaker workbook as a surrogate acute oral RfD of 0.413 mg/kg bw and a chronic oral RfD of 0.02 mg/kg bw. Both studies identify effects on the kidneys as the most sensitive endpoint. In addition, both of the RfDs use an uncertainty factor of 100—i.e., a factor of 10 for extrapolation from animals to humans and a factor of 10 for potentially sensitive individuals.

The EPA did not derive a single dose acute RfD because studies documenting an adverse effect from a single dose were not identified (U.S. EPA/OPP/HED 2012).

The surrogate acute RfD used in the current analysis is based on a 90-day oral toxicity study in mice with a NOAEL of 41.3 mg/kg bw/day and a corresponding LOAEL of 113 mg/kg bw/day. This study is not identified explicitly in U.S. EPA/OPP/HED (2012) but is used to characterize risks associated with short-term (1-30 days) oral exposures. U.S. EPA/OPP (1999a, p. 224) identifies several 90-day studies in rodents but does not explicitly discuss a 90-day study in mice with an NOAEL of 41.3 mg/kg bw/day.

The chronic RfD is based on chronic dietary study in rats exposed to doses of 0, 2, 4, 15 or 175 mg/kg/day for 23-29 months (MRID 41250502). No effects were noted at 2 mg/kg bw/day, but effects on the kidney as well as ulcers and forestomach hyperplasia were noted at 4 mg/kg bw/day. This study is not detailed in U.S. EPA/OPP/HED (2012) but is discussed in some detail in the EPA RED for chlorothalonil (U.S. EPA/OPP 1999a). The chronic RfD of 2 mg/kg bw/day noted in the most recent EPA human health risk assessment (U.S. EPA/OPP/HED 2012) is identical to the chronic RfD in the RED (U.S. EPA/OPP 1999a).

3.3.2. Inhalation Toxicity

U.S. EPA/OPP/HED (2012) derives acute (1 day) and short-term/intermediate (1-30 days/ 1-6 months) inhalation toxicity values for chlorothalonil. Both values are based on an acute inhalation study in rats which identified a LOAEL of 0.002 mg/L (2,000,000 ng/m^3) based on … *hypoactivity, gasping, lacrimation, nasal discharge, piloerection, ptosis (eyelid droop), and respiratory gurgle* (U.S. EPA/OPP/HED 2012, p. 29). The specific study is not identified or referenced explicitly in U.S. EPA/OPP/HED (2012). Based on this LOAEL, the EPA derives Human Equivalent Concentrations (HECs) of 0.0004 mg/L for acute exposures and 0.00006 mg/L for short-term/intermediate exposures. U.S. EPA/OPP/HED (2012) does not detail the derivation of these values; presumably they follow standard methods used by the EPA in the derivation of inhalation reference concentrations (RfCs)—e.g., U.S. EPA/ORD (1994).

For acute exposures, U.S. EPA/OPP/HED (2012) recommends a Margin of Exposure (MOE) of 100. Thus, the HEC of 0.0004 mg/L and MOE of 100 is equivalent to an RfC of 0.000004 mg/L [0.0004 mg/L ÷ 100].

For short-term/intermediate exposures, U.S. EPA/OPP/HED (2012) recommends a Margin of Exposure (MOE) of 1000. Thus, the HEC of 0.00006 mg/L and MOE of 1000 is equivalent to an RfC of 0.00000006 mg/L [0.00006 mg/L ÷ 1000].

3.4. Risk Characterization

3.4.1. Workers

3.4.1.1. Standard Exposure Scenarios

The risk characterization for workers is given in Worksheet E02. The HQs for general exposures (i.e., exposures anticipated in the normal application of chlorothalonil) are 0.02 (0.0003-0.5). Worker exposures are below the level of concern by a factor of 50 based on the central estimate and below the level of concern by a factor of 2 based on upper bounds.

The only accidental exposure scenario resulting in HQs that exceed the level of concern (HQ=1) is the scenario for wearing contaminated gloves for 1 hour. For this scenario are HQs are 7 (3 to 15).

3.4.1.2. Inhalation Exposure Scenarios

As summarized in Table 3, acute and longer-term HQs can be derived based on the monitoring data and toxicity value from U.S. EPA/OPP/HED (2012). While the acute HQs are below the level of concern (HQ=1), some of the chronic HQs exceed the level of concern by factors of up to about 5. Since the toxicity values are based on a LOAEL (Section 3.3), an elaboration of the HQs based on considerations of the NOAEL to the LOAEL cannot be made.

As discussed in Section 3.2.1.3, the monitoring data are not associated explicitly with application rates and proximity to the treated area during or after application. Consequently, the relevance of the exceedances to Forest Service activities is difficult to assess. In addition, as noted by the EPA, the limited toxicity data—i.e., one acute inhalation bioassay—makes any risk characterization tenuous. In addition, the EPA notes that there are no reports of adverse effects following inhalation exposures to chlorothalonil.

> *Based on the lack of incident data related to inhalation effects and the fact that an acute inhalation toxicity study is being used to assess short-and intermediate-term risk, the risk assessment can be characterized as conservative.*
>
> U.S. EPA/OPP/HED 2012, p. 16

In the absence of additional relevant toxicity data and a more refined exposure assessment, the risk characterization associated with potential inhalation exposures during or following applications of chlorothalonil cannot be elaborated.

3.4.2. General Public

The risk characterization for members of the general public is given in Worksheet E04. Based on standard exposure scenarios for forestry applications, some of the HQs for the consumption of contaminated vegetation exceed the level of concern with upper bound HQs of up to 7 for acute exposures and 66 for longer-term exposures. The extent to which these exposures are relevant to a nursery application should be evaluated further.

HQs for the consumption of contaminated fish following an accidental spill exceed the level of concern with upper bound HQs of 11 for the general public and 52 for subsistence populations. In the event of an accidental spill, measures to limit exposures in members of the general public and subsistence populations would be warranted.

4. ECOLOGICAL EFFECTS

4.1. Hazard Identification

As noted in Section 3.1, the mechanism of fungicidal activity of chlorothalonil involves an inhibition of glycolysis. As discussed by U.S. EPA/OPP/EFED (2012, p. 56), chlorothalonil is toxic to fungi as well as algae and bacteria; however, the mechanism of action in algae and bacteria has not been characterized. Information regarding the mechanism of action in other nontarget species was not identified in the available literature.

U.S. EPA/OPP/EFED has identified 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene, an environmental metabolite of chlorothalonil and an agent of toxicological concern referred to as SDS-3701 (U.S. EPA/OPP/EFED 2012, p. 16). As illustrated in Table 1, SDS-3701 is a hydroxylated metabolite of chlorothalonil in which the 4-chlorine is replaced by a hydroxyl group (-OH). This compound is also referred to as chlorothalonil-4-hydroxy (http://www.chemicalbook.com/ChemicalProductProperty_EN_CB9505982.htm). While SDS-3701 is less acutely toxic than chlorothalonil to aquatic species, this metabolite is more acutely toxic than chlorothalonil to mammals and birds (U.S. EPA/OPP/EFED 2012, p. 36). Consequently, U.S. EPA/OPP/EFED (2012) explicitly considers exposures to both chlorothalonil and SDS-3701 in the assessment of risks to mammals and birds.

Appendix G of U.S. EPA/OPP/EFED (2012) provides additional details (e.g., NOAECs) that are useful in the current assessment. In the interest of brevity, this appendix is sometimes cited simply as "EPA Appendix G" in the following discussion.

4.2. Exposure Assessment

4.2.1. Bioconcentration

As discussed in Section 3.2.2.3 and summarized in Table 1, BCF values used in the ecological risk assessment are 3041 for acute exposure scenarios and 3077 for longer-term exposure scenarios.

4.2.2. Offsite Contamination of Soil

Rates for the offsite contamination of soil are typically handled in full or scoping level Forest Service risk assessments using GLEAMS-Driver modelling. In the interest of economy, the current effort uses a central estimate of 5% with a range of 1% to 10% of the nominal application rate). These values are similar to estimates of offsite losses noted in Forest Service pesticide risk assessments as well as assumptions often used in EPA risk assessments.

4.2.3. Exposures to SDS-3701

As detailed in SERA (2014a), most Forest Service risk assessments are based on a series of exposure assessments for mammals, birds, terrestrial invertebrates, plants, and aquatic organisms. These exposure assessments are detailed in the WorksheetMaker book that accompanies this document. Details of and the rational for these exposure assessments are given in Section 4.2 of SERA (2014a) and not discussed further in the current document. One exception, however, involves terrestrial plants. Because standard toxicity studies are not available on terrestrial plants, standard exposure assessments for terrestrial plants are not given in the WorksheetMaker workbook that accompanies this document.

As noted in Section 4.1, U.S. EPA/OPP/EFED considers the metabolite 4-hyrdroxy-chlorothalonil (SDS-3701) as a metabolite of concern for birds and mammals (U.S. EPA/OPP/EFED 2012). In estimating exposures to SDS-3701 in contaminated vegetation, the EPA multiplies the dose of chlorothalonil by a factor of 0.3174 to approximate the dose of SDS-3701. This factor is based on observations that maximum residues of SDS-3701 are a fraction of 0.341 of the maximum residue of chlorothalonil with a correction for the molecular weight of SDS-3701 (247.5 g/mole) relative to chlorothalonil (265.9 g/mole) [(247.5/265.9) x 0.341 ≈ 0.31740316].

In addressing the impact of SDS-3701 on risks to mammals and birds, U.S. EPA/OPP/EFED (2012, e.g., Table 5-7) provides separate RQs (risk quotients) associated with chlorothalonil and SDS-3701. As discussed in the documentation for WorksheetMaker (SERA 2011a, Section 3.4.3), a utility is available in WorksheetMaker for assessing exposures to mixtures by combining workbooks. Because the consideration of SDS-3701 involves only mammals and birds, the current analysis takes a conceptually similar approach that is somewhat easier to implement.

Adopting the conservative assumption of simple similar action from Finney (1972), adjustment factors are developed for deriving doses of chlorothalonil that are equivalent to combined exposures to chlorothalonil and SDS-3701. This factor is then applied to a downward adjustment to the toxicity value for chlorothalonil which accounts for the joint exposure to SDS-3701. In deriving this factor, relative potency is determined as the ratio of equitoxic doses of chlorothalonil and SDS-3701. In the applications discussed in Section 4.3.1, NOAELs are used as equitoxic doses. Thus, the potency (ρ) of SDS-3701 relative to chlorothalonil is defined as:

$$\rho = \frac{NOAEL_{Chlorothalonil}}{NOAEL_{SDS-3701}} \quad (1)$$

Based on this definition of potency, a dose of SDS-3701 can be converted to an equivalent dose of chlorothalonil by multiplying the dose of SDS-3701 by the potency. Based on this conversion, adjustment factors for the toxicity value of chlorothalonil can be developed as detailed in Section 4.3.1.

4.3. Dose-Response Assessment

The dose response assessment for nontarget organisms is summarized in Table 6 and is discussed in the following subsections on different groups of receptors.

4.3.1. Terrestrial Organisms

4.3.1.1. Mammals

4.3.1.1.1. Acute Toxicity

Forest Service risk assessments typically use the acute NOAEL from the human health risk assessment that forms the basis of the acute RfD. As summarized in Table 5 and discussed in Section 3.3, the acute NOAEL is 41.3 mg/kg bw/day.

As discussed in Section 4.2.3, a complicating factor to the dose-response assessment for chlorothalonil involves co-exposure to SDS-3701. For SDS-3701, U.S. EPA/OPP/EFED (2012, e.g., Table 5-7) uses the acute LD_{50} of 242 mg/kg bw for SDS-3701. Following the standard approach used in Forest Service risk assessments (SERA 2014a, Section 4.3.2), the LD_{50} is divided by a factor of 10 to approximate a NOAEL of 24.2 mg/kg bw. Following the approach discussed in Section 4.2.3, the potency of SDS-3701, relative to chlorothalonil, is estimated as 1.7 [41.3 mg/kg bw ÷ 24.2 mg/kg bw ≈ 1.70661].

As discussed in Section 4.2.3, the exposure to SDS-3701 will be a fraction of 0.3174 of the nominal exposure to chlorothalonil. Correcting for the loss of chlorothalonil in conversion to SDS-3701, the actual exposure to chlorothalonil will be 0.6826 [1-0.3174] of the nominal exposure chlorothalonil. Adjusting for relative potency, the combined exposure to the two compounds will be equal to about 1.2 [0.6826 + (1.7 x 0.3174) ≈ 1.22218] equivalents of chlorothalonil. In other words, the plausible simultaneous exposures to chlorothalonil and SDS-3701 will be more toxic than the anticipated single exposure to chlorothalonil by a factor of 1.2. To account for this difference, the acute NOAEL of 41.3 mg/kg bw/day is divided by a factor of 1.2, and an adjusted NOAEL of 34.3 mg/kg bw is used for chlorothalonil.

As an illustration and check of the above calculations, note that the adjustment of the NOAEL for chlorothalonil to 34.3 mg/kg is equivalent to stating that an exposure to the nominal dose of chlorothalonil of 34.3 mg/kg is equivalent to the level of concern (HQ=1) if the co-exposure to SDS-3701 is considered. If 0.3174 of chlorothalonil is converted to SDS-3701, the dose of chlorothalonil apart from SDS-3701 is about 23.5 mg/kg bw [34.3 mg/kg x (1-0.3174) ≈ 23.49282 mg/kg bw] and the dose of SDS-3701 is about 10.9 mg/kg bw [34.3 mg/kg x 0.3174 ≈ 10.92385 mg/kg bw]. Taking the NOAELs of 41.3 mg/kg bw for chlorothalonil and 24.2 mg/kg bw for SDS-3701, the HQs are about 0.57 for chlorothalonil [23.5÷41.3 ≈ 0.569] and 0.45 for SDS-3701 [10.9 ÷ 24.2 ≈0.450]. The combined HQ (often referred to as a hazard index) is equal to about 1.0 [0.57 + 0.45 = 1.02]. The slight variance from 1 is due completely to rounding values in the calculations.

4.3.1.1.2. Chronic Toxicity

For chronic toxicity, the longer-term NOAEL for the chronic RfD is 2 mg/kg bw/day (Table 5 with a discussion in Section 3.3). U.S. EPA/OPP/EFED (2012, Table 5-7, p. 158) notes that no data are available on the chronic toxicity of SDS-3701 and the EPA does not quantitatively consider the effect of longer-term exposures to SDS-3701. The current document adopts this approach, and the chronic NOAEL for chlorothalonil is taken as 2 mg/kg bw/day.

If an adjustment for longer-term exposures to SDS-3701 were to be made, an acute-to-chronic ratio approach would lead to the same adjustment used for acute toxicity (Section 4.3.1.1.1).

4.3.1.2. Birds

4.3.1.2.1. Acute Toxicity

The approach to the acute toxicity of chlorothalonil in birds is essentially the converse of the approach used for chronic toxicity in mammals. As noted in U.S. EPA/OPP/EFED (2012, Table 5-9, p. 156), all of the acute toxicity values for chlorothalonil in birds are indefinite—i.e., all of the acute oral LD_{50} values and acute dietary LC_{50} values are reported as "greater than" the

highest dose tested. Consequently, the acute toxicity of chlorothalonil is not considered explicitly.

For SDS-3701, the lowest acute oral LD_{50} is 158 mg/kg bw and the lowest acute dietary LC_{50} is 1746 ppm (mg SDS-3701/kg diet) with an NOEL of 562 ppm based on a bioassay in quail (MRID 00115109, as detailed in U.S. EPA/OPP/EFED 2012, Appendix G, p. 3). Taking a consumption rate of 0.3 kg chow/kg bw for quail (SERA 2007a), the NOAEL of 562 ppm is equivalent to dose of 168.6 mg SDS-3701/kg bw [562 mg SDS-3701/kg chow x 0.3 kg chow/kg bw ≈ 168.6 mg/kg bw]. Taking a factor of 0.3174 to approximate the dose of SDS-3701 from chlorothalonil, the equivalent dose of chlorothalonil is taken as about 530 mg/kg bw [168.6 mg/kg bw ÷ 0.3174 ≈ 531 mg/kg bw]. Thus, the functional NOAEL for chlorothalonil used in the WorksheetMaker workbook for birds is 530 mg/kg bw.

4.3.1.2.2. Chronic Toxicity

For chronic toxicity to birds, NOAELs are available for both chlorothalonil and SDS-3701. As summarized in U.S. EPA/OPP/EFED (2012, Table 5-9, p. 156) with additional details in EPA Appendix G (Table G.1-4, p. 3), the most sensitive longer-term NOAEL for birds is 153 mg/kg chow in a quail study (MRID 45710218). Similarly, the most sensitive endpoint for birds is a longer-term NOAEL of 50 mg/kg chow for mallards (U.S. EPA/OPP/EFED 2012, Appendix G, Table G.1-5, p. 5 of Appendix G, MRID 40729402). Using a food consumption rate of 0.07 chow/kg bw for longer-term studies in quail and mallards (SERA 2007b), these toxicity values correspond to about 11 mg/kg bw/day for chlorothalonil [153 mg/kg chow x 0.07 chow/kg bw/day ≈ 10.71 mg /kg bw] and 3.5 mg/kg bw/day for SDS-3701 [50 mg/kg chow x 0.07 chow/kg bw = 3.5 mg/kg bw/day].

Following the same general approach used for acute toxicity in mammals (Section 4.3.1.1.1), the potency of SDS-3701, relative to chlorothalonil, is about 3.1 [11 mg/kg bw/day ÷ 3.5 mg/kg bw/day ≈ 3.142857]. Again using 0.3174 as the proportion of chlorothalonil converted to SDS-3701, correcting for the loss of chlorothalonil in conversion to SDS-3701, and adjusting for relative potency, the combined exposure to the two compounds will be equal to about 1.7 [0.6826 + (3.1 x 0.3174) ≈ 1.66654] equivalents of chlorothalonil. Thus, the NOAEL of 11 mg/kg bw/day for chlorothalonil, not considering SDS-3701, is adjusted to 6.5 mg/kg bw/day [11 mg/kg bw/day ÷ 1.7 ≈ 6.471 mg/kg bw/day] to consider co-exposures to SDS-3701.

4.3.1.3. Other Terrestrial Organisms

4.3.1.3.1. Honeybee

U.S. EPA/OPP/EFED did not calculate risk quotients for the honeybee because all LD_{50} values were non-definitive (U.S. EPA/OPP/EFED 2012, p. 158) As summarized in Appendix G (p.9) of the EPA risk assessment, a dose of 181 µg/bee is associated with 14.28% lethality, and chlorothalonil is classified as 'Practically non-toxic' to the honeybee (MRID 00036935). No details of this study are provided, and it is not clear if the noted mortality was significantly different from control mortality. In another study (MRID 00077759), a dose of 181 µg/bee was noted to be non-toxic to the honeybee.

For the current assessment, 181 µg/bee is taken as a marginal NOAEL. Using a typical body weight of 116 mg (equivalent to 0.000116 kg) for a worker bee (SERA 2014a, Section 4.2.3.1),

the dose of 0.181 mg/bee is equivalent to about 1560 mg/kg bw [0.181 mg/bee ÷ 0.000116 kg bw ≈ 1560.3448 mg/kg bw].

No oral toxicity data for the honeybee is given in U.S. EPA/OPP/EFED (2012).

4.3.1.3.2. Terrestrial Plants

As summarized in U.S. EPA/OPP/EFED (2012, p. 178), a quantitative risk assessment for terrestrial plants was not conducted because of the very low toxicity of chlorothalonil to terrestrial plants—i.e., NOAEL > 16 lb a.i./acre. Note that the NOAEL is indefinite—i.e., a LOAEL is not identified. The current document maintains consistency with EPA, and the toxicity of chlorothalonil to terrestrial plants is not further considered.

4.3.2. Aquatic Organisms

As discussed in the following sections, most acute toxicity values are reported in U.S. EPA/OPP/EFED (2012) in units of µg/L. In the WorksheetMaker workbook that accompanies this report, toxicity values are expressed in units of mg/L. In the following sections, toxicity values are generally discussed in units of µg/L to maintain consistency with the EPA source document. All toxicity values used in the WorksheetMaker workbook, however, are also expressed in units of mg/L (usually parenthetically) for clarity.

4.3.2.1 Fish

4.3.2.1.1 Acute Toxicity

U.S. EPA/OPP/EFED (2012, Appendix G, Section G.4.1, pp. 10-13) summarizes several acute toxicity studies in fish with reported LC_{50} values for technical grade chlorothalonil ranging from 10.5 µg a.i./L for rainbow trout to 120 µg a.i./L for tilapia (EPA Appendix G, Table G.4-2, Ecotox No. 87454; 7055). For formulated chlorothalonil, LC_{50} values range from 32 to 125 µg a.i./L. Based on these toxicity values, chlorothalonil is classified as "very highly toxic to highly toxic" to fish. Two acute LC_{50} values are reported for SDS-3701—i.e., 15,000 to 45,000 µg/L (EPA Appendix G, Table G.4-4), and SDS-3701 is classified as slightly toxic. Given the substantially greater potency of chlorothalonil to fish, relative to SDS-3701, SDS-3701 is not further considered quantitatively. This approach is consistent with the approach used in U.S. EPA/OPP/EFED (2012, Table 5-1, pp. 146-147).

As in EPA/OPP/EFED (2012, Table 5-1, p. 147), the LC_{50} for sensitive species of fish is taken as 10 µg a.i./L. In the absence of a reported NOAEC, the LC_{50} is divided by 20 to approximate a NOAEC of 0.5 µg a.i./L (0.0005 mg a.i./L). The rationale for this approach (which also applies to other aquatic organisms) is discussed in SERA (2014a, Section 4.3.2 and Table 19).

The NOAEC for tolerant species of fish is based on an LC_{50} of 120 µg a.i./L, the highest reported LC_{50} reported in U.S. EPA/OPP/EFED (2012). Dividing by 20, the NOAEC is estimated at 6 µg a.i./L (0.006 mg/L).

4.3.2.1.2 Chronic Toxicity

U.S. EPA/OPP/EFED (2012, Table 5-1, p. 147) uses a longer-term (60-day) NOAEC of 1.3 µg/L. As detailed in U.S. EPA/OPP/EFED (2012, Appendix G, Section G.4.6, pp. 13-14), this NOAEC is from an early life state study in fathead minnow (MRID 00030391) in which adverse effects (decreased egg production) were noted at 2.9 µg a.i./L. No acute toxicity data are

available for fathead minnow. Consequently, the NOAEL of 1.3 µg/L is applied to presumably tolerant species, and a dose-response assessment for potentially sensitive species is not developed.

4.3.2.2. Amphibians (Aquatic phase)

While the U.S. EPA/OPP/EFED (2012, Appendix G, Section G.4.7) summarizes some data on the effects of chlorothalonil on amphibians, these data are not used in the main body of the U.S. EPA/OPP/EFED (2012, Table 5-1) risk assessment to quantitatively assess risks to amphibians. The current document adopts the same approach, and risks to fish are used as surrogates for aquatic phase amphibians.

4.3.2.3. Aquatic Invertebrates

4.3.2.3.1. Sensitive Species

For aquatic invertebrates, U.S. EPA/OPP/EFED (2012, Table 5-2, p. 149) use *Daphnia magna* as a surrogate species. For acute toxicity, the EPA characterizes risk with an acute LC_{50} of 54 µg a.i./L and chronic toxicity with a NOAEC of 0.6 µg a.i./L. As detailed in U.S. EPA/OPP/EFED (2012, Appendix G), the acute LC_{50} is from a registrant-submitted study (Table G.4-6, p. 16). The chronic NOAEC is also from a registrant-submitted study in which the LOAEC is 1.8 µg/L based on survival (MRID 45710222). The EPA expresses concern with the chronic study:

> *Because chlorothalonil concentrations declined to less than the level of detection at the lower concentrations, there is uncertainty in the chlorothalonil levels associated with toxic effects in this study.*
>
> U.S. EPA/OPP/EFED (2012, Appendix G, p. 19).

Following standard practice in Forest Service risk assessment (SERA 2014a), LC_{50} values are not used directly in risk characterization. In the absence of a reported NOAEC, the acute LC_{50} is divided by a factor of 20 (SERA 2014a, Section 4.3.2 and Table 19) to approximate an acute NOAEC of 2.7 µg a.i./L [54 µg a.i./L ÷ 20 = 2.7 µg a.i./L]. This value is higher than the chronic NOAEC of 0.6 µg/L. Thus, for the current analysis, the acute NOAEC is taken as 2.7 µg a.i./L (0.0027 mg a.i./L) and the longer-term NOAEC is taken as 0.6 µg a.i./L (0.0006 mg a.i./L).

4.3.2.3.2. Tolerant Species

U.S. EPA/OPP/EFED (2012, Appendix G) provides a brief summary of a registrant-submitted study in which acute LC_{50} values of up to 1600 µg a.i./L are reported (Table G.4-6, p. 16, MRID 4341601). This study is classified as supplemental; however, some of the deficiencies in this study noted by EPA are substantial—i.e., *negative control not used, unacceptable control mortality; prior exposure to field collected organisms unknown (acclimation unknown); potential cannibalism*. The EPA also summarizes several open literature studies in which EC_{50} values for chlorothalonil up to 280 µg a.i./L (freshwater mussel, *Lampsilis siliquoidea*) are reported.

For the current analysis, the EC_{50} of 280 µg a.i./L is divided by 20 to approximate an acute NOAEC of 14 µg a.i./L [280 µg a.i./L ÷ 20 = 14 µg a.i./L] (0.014 mg a.i./L).

No chronic studies on species other than daphnids are reported in U.S. EPA/OPP/EFED (2012, Appendix G). Consequently, longer-term risks to tolerant species of aquatic invertebrates are not characterized. A more refined analysis could approximate longer-term NOAECs for aquatic species using the relative potency method. Since the open literature studies were not reviewed as part of the current analysis, this approach does not seem justified.

4.3.2.4. Aquatic Plants

4.3.2.4.1. Algae

4.3.2.4.1.1. Sensitive Species

For sensitive species of nonvascular aquatic plants, U.S. EPA/OPP/EFED (2012, Table 5-4, p. 152) uses an IC_{50} (i.e., concentration associated with 50% inhibition, essentially identical to an EC_{50}) of 12 µg a.i./L. This concentration appears to be the lower bound of the EC_{50} for chlorothalonil in *Navicula pelliculosa*, a freshwater diatom (EPA Appendix G, Table G.5.2, p. 23, MRID 44908105). The NOAEC from this study is reported as 3.9 µg a.i./L (0.0039 mg a.i./L) and is used in the risk characterization for sensitive species of algae.

4.3.2.4.1.2. Tolerant Species

U.S. EPA/OPP/EFED (2012, Appendix G, Table G.5.2, p. 23) reports an additional NOAEC of 50 µg a.i./L in a species of green algae, *Selenastrum capricornutum* (MRID 42432801). Additional open literature studies are also reviewed (EPA Appendix G.5-3, p. 24), but NOAECs are not identified.

In the absence of additional information, the NOAEC of 50 µg a.i./L (0.050 mg/L) is used to characterize risks in tolerant species of algae.

4.3.2.4.2. Aquatic Macrophytes

U.S. EPA/OPP/EFED (2012, Table 5-5, p. 153) uses an EC_{50} of 640 µg a.i./L to characterize risks in aquatic macrophytes. As summarized in EPA Appendix G (Table G.5-2, pp. 22-23), this EC_{50} comes from a study in a species of duckweed (*Lemna gibba*) which also noted a NOEC of 290 µg a.i./L.

This is the only information encountered on the toxicity of chlorothalonil to aquatic plants. In the absence of additional information, the NOEC of 290 µg a.i./L (0.29 mg/L) is applied to presumably tolerant species.

4.4. Risk Characterization

4.4.1. Terrestrial Organisms

4.4.1.1. Mammals

The risk characterization for mammals is summarized in Worksheet G02a. As with the human health risk assessment for members of the general public (Worksheet E03), the major concern involves small mammals consuming contaminated vegetation with upper bound HQs of up to 24 for acute exposures and 339 for longer-term exposures. Exposures associated with contaminated water are below the level of concern, except for the consumption of contaminated fish following an accidental spill.

4.4.1.2. Birds

The risk characterization for birds is summarized in Worksheet G02b. As with mammals, the exposure scenarios associated with HQs that exceed the level of concern involve the consumption of contaminated vegetation. For birds, however, the HQs are lower than for mammals with upper bound HQs of 7 for acute exposures and 258 for longer-term exposures.

4.4.2. Aquatic Organisms

The risk characterization for aquatic organisms is summarized in Worksheet G03. An accidental spill of chlorothalonil could cause substantial damage to all groups of aquatic organisms. Non-accidental acute exposures exceed the level of concern for sensitive and tolerant species of fish as well as sensitive species of aquatic invertebrates and algae.

5. REFERENCES

5.1. Chemical Specific References

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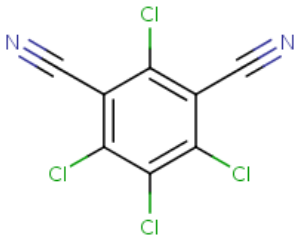
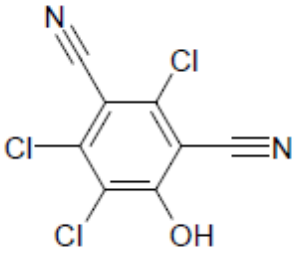
Table 1: Chemical and Physical Properties

Item	Value	Reference[1]
	Identifiers	
Common name:	chlorothalonil	
CAS Name	2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile	Tomlin 2004
CAS No.	1897-45-6	ChemIDplus 2014
Chemical Group	Chlorinated aromatic	ChemIDplus 2014
Development Codes	DS-2787 (Diamond Shamrock)	Tomlin 2004
IUPAC Name	tetrachloroisophthalonitrile	Tomlin 2004
Molecular formula	$C_8Cl_4N_2$	Tomlin 2004
Mechanistic group	Fungicide, disruption of glycolysis	Tomlin 2004
EPA PC Code		
Smiles Code	`Clc1c(Cl)c(C#N)c(Cl)c(C#N)c1Cl`	Tomlin 2004
	`c1(c(c(c(Cl)c(c1Cl)Cl)C#N)Cl)C#N`	ChemIDplus 2014
Smiles Code with stereochemistry		
Structure of chlorothalonil		ChemIDplus 2014
Structure of 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (a.k.a. SDS-3701 or 4-hydroxy-chlorothalonil) CAS: 28343-61-5 MW: 247.5		U.S. EPA/OPP/EFED 2012, p. 37 http://www.chemicalbook.com/ChemicalProductProperty_EN_CB9505982.htm See Section 4.1 for discussion.
	Chemical Properties(1)	
Aqueous photolysis	10.3 hour half-life at pH 7	U.S. EPA/OPP/EFED 2012, Table 2-2, MRID 45710223
	0.4 days	EPA/OPP/EFED 2012, Table 3-1
Boiling point	350 °C/760 mm Hg	Tomlin 2004
Henry's Law Constant	2.50×10^{-2} Pa m^3 mol^{-1} (25 °C)	Tomlin 2004
Hydrolysis	Stable	U.S. EPA/OPP/EFED 2012, Table 2-2, MRID 00040539 and Table 3-2
K_{ow}	≈832 [logP = 2.92]	Tomlin 2004
	≈1,122[logP = 3.05]	ChemIDplus 2014
	≈6,309[logP = 3.8] – value used in workbook.	U.S. EPA/OPP/EFED 2012, p. 117.
Molecular weight	265.9 g/mole	Tomlin 2004; U.S. EPA/OPP/EFED 2012, Table 3-1
Melting point	252.1 °C	Tomlin 2004
Vapor pressure	0.076 mPa (25 °C)	Tomlin 2004
Water solubility	0.81 mg/l (25 °C)	Tomlin 2004

<table>
<tr><th>Item</th><th>Value</th><th>Reference[1]</th></tr>
<tr><td></td><td>0.8 mg/l – value used in workbook.</td><td>EPA/OPP/EFED 2012, Table 3-1</td></tr>
<tr><td></td><td colspan="2">Environmental Properties</td></tr>
<tr><td>Aerobic aquatic metabolism</td><td>0.06 to 3.4 days (first-order)</td><td>U.S. EPA/OPP/EFED 2012, Table 2-2, several studies</td></tr>
<tr><td></td><td>1.5 days (upper 90th percentile confidence bound on the mean value of 2.6, 1.4, 0.8, 0.3, 0.1, and 0.1 days).

Recalculated Mean and 80% confidence interval: 0.88 (0.29 to 1.47) days. See Appendix 2, Table A2-2, of the current report.</td><td>U.S. EPA/OPP/EFED 2012, Table 3-2, several studies</td></tr>
<tr><td>Anaerobic aquatic metabolism</td><td>9.7 and 10.6 days (first-order)</td><td>U.S. EPA/OPP/EFED 2012, Table 2-2, MRID 00147975</td></tr>
<tr><td></td><td>11.5 days (upper 90th percentile confidence bound on mean value of 8.9 and 4.8 days)</td><td>U.S. EPA/OPP/EFED 2012, Table 3-3, several studies</td></tr>
<tr><td>Bioconcentration in fish (BCF)</td><td><table><tr><th>Initial Water Conc.</th><th>BCF (edible)</th><th>BCF (whole fish)</th></tr><tr><td>0.1 µg/L</td><td>256</td><td>3077</td></tr><tr><td>0.5 µg/L</td><td>306</td><td>3041</td></tr></table></td><td>U.S. EPA/OPP/EFED 2012, Table 2-2, MRID 45710224</td></tr>
<tr><td>Bioconcentration in whole oyster (BCF)</td><td>2660 (total residue primarily of transformation products)</td><td>U.S. EPA/OPP/EFED 2012, Table 2-2, MRID 43070601</td></tr>
<tr><td>Field dissipation, half-lives</td><td>58, 56, 74, and 81 days</td><td>U.S. EPA/OPP/EFED 2012, Table 2-2, MRID 00071625</td></tr>
<tr><td></td><td>33, 46, 50, 58, and 74 days</td><td>U.S. EPA/OPP/EFED 2012, Table 2-2, several studies</td></tr>
<tr><td>Foliar washoff fraction</td><td>0.5</td><td>Knisel and Davis 2000</td></tr>
<tr><td>Foliar half-life</td><td>10 days</td><td>Knisel and Davis 2000</td></tr>
<tr><td></td><td>35 days (highest value from Willis and McDowell 1987)</td><td>U.S. EPA/OPP/EFED 2012, Table 3-4, default value</td></tr>
<tr><td></td><td>4.1 ± 1.5 days (apples)</td><td>Willis and McDowell 1987</td></tr>
<tr><td>K_{oc}</td><td>1121, 2039, 2958, 5085, 6605, and 11935 mL/g OC</td><td>U.S. EPA/OPP/EFED 2012, Table 2-2, MRID 00029406</td></tr>
<tr><td></td><td>Central estimate of 4040 from MRID 00029406</td><td>EPA/OPP/EFED 2012, Table 3-1</td></tr>
<tr><td></td><td>1380</td><td>Knisel and Davis 2000</td></tr>
<tr><td></td><td>1600 (sand); 14,000 (silt)</td><td>Tomlin 2004</td></tr>
<tr><td>Soil half-life, aerobic metabolism</td><td>Reported first-order half-lives of 0.3 to 58 days. Other more complex kinetic models also considered.</td><td>U.S. EPA/OPP/EFED 2012, Table 2-2 several studies</td></tr>
<tr><td></td><td>16 days (90th percentile of 57, 22, 18, 15, 14, 10, 10, 5, 2, 1, 1, 1, 0.5, 0.3 days)
Recalculated Mean and 80% confidence interval: 11.2 (5.76 to 16.64) days. See Appendix 2, Table A2-1.</td><td>U.S. EPA/OPP/EFED 2012, Table 3-3, several studies</td></tr>
<tr><td>Soil photolysis</td><td>Stable</td><td>U.S. EPA/OPP/EFED 2012, Table 2-2, MRID 00087349 and MRID 00040543</td></tr>
</table>

See Section 2 for discussion.

Table 2: Derivation of Worker Exposure Rates for Broadcast Applications

Item	Value	Reference/Note	Row
Reference Chemical	2,4-D	Section 3.2.1	2
First-order dermal absorption rate coefficient for reference chemical ($hour^{-1}$) [ka_{Ref}]	0.00066	SERA 2014b	3
Occupational Exposure Rates for Reference Chemical			4
Central Estimate	0.0001	SERA 2014b, Table 14	5
Lower 95% Prediction Bound	0.000002	SERA 2014b, Table 14	6
Upper 95% Prediction Bound	0.005	SERA 2014b, Table 14	7
Subject Chemical	Chlorothalonil		8
First-order dermal absorption rate coefficient for subject chemical ($hour^{-1}$) [ka_P]	0.00019	Section 3.2.1.	9
$ka_P \div ka_{Ref}$	0.2878787879		10
Occupational Exposure Rates for Reference Chemical			11
Central Estimate	0.0000287879	SERA 2014b, Eq. 22	12
Lower 95% Prediction Bound	0.0000005758	SERA 2014b, Eq. 22	13
Upper 95% Prediction Bound	0.0014393939	SERA 2014b, Eq. 22	14

See Section 3.2.1. for discussion.

Documentation for Table: The above table implements the adjustment of worker exposure rates based dermal absorption rates. The table uses MS Word "fields" rather than macros.

- Determine the first-order dermal absorption rate coefficient for the chemical under review. See SERA 2014a, Section 3.1.3.2.2.
- Select the reference chemical. See SERA 2014b, Section 4.1.6.1.
- Fill in the information on the reference chemical in the upper section of the above table.
- Fill in the first-order dermal absorption rate coefficient for the chemical under review in the Value column of Row 9 in the above table.
- Update the estimated values for ration of the k_a values and the occupational exposure rates for the chemical under review – i.e., the green shaded cells in the above table. The simplest way to update these fields is to select each of the 4 green shaded cells (one at a time and in order), press the right mouse button, and select 'Update field'.

Assuming that you will construct an EXCEL workbook, it is a good idea to check the above calculations in EXCEL. Also note that you should round the values in the green shaded cells to one significant figure in the EXCEL workbook if you want to maintain compatibility with SERA (2014b).

Table 3: Inhalation Exposures at Application Sites

Study	Year	Location	Max. Conc. (ng/m3)	Mean Conc. (ng/m3)	Acute HQ	Longer-term HQ
San Joaquin County, CA	2002	North	70	32	0.0175	0.533
		Northeast	83	45	0.0208	0.75
		East	737	324	0.184	**5.4**
		Southeast	413	262	0.103	**4.4**
		Southeast	296	198	0.074	**3.3**
		Southwest	80	36	0.020	0.6
		West	372	127	0.093	**2.1**
		Northwest	29	17	0.00725	0.28
Ventura County, CA	1992	East Site 1	158	74	0.0395	**1.2**
		East Site 2	58	28	0.0145	0.46
		West Sites 1 and 2	23	23	0.00575	0.38

Toxicity Values			
Acute RfC	4,000	ng/m3	Table 5 in this document
Longer-term RfC	60	ng/m3	Table 5 in this document

Source: U.S. EPA/OPP/HED 2012, Table A5.4, p. 44
See Section 3.2.1.3 for discussion of exposure.
See Section 3.4.1.2 for discussion of risk characterization.

Table 4: Inputs and Outputs for FIRST Simulations

Parameter	Central Estimate of Concentration in Water	Lower Bound of Concentration in Water	Upper Bound of Concentration in Water
Aerobic soil metabolism half-life (days) [1]	11.2	5.76	16.64
Aerobic aquatic metabolism (days) [2]	0.88	0.29	1.47
K_{oc} (mL/g) [3]	4040	11,935	1121
Photolysis half-life (days) [4]	0.4	0.4	0.4
Water solubility (mg/L) [4]	0.8	0.8	0.8
Gross Peak Concentration (µg/L)	20.6	15.7	34.9
Gross Longer-term Concentration (µg/L)	0.237	0.157	0.383
Proportion of Treated Watershed	0.14		
Peak Concentration Used in Analysis (µg/L)	2.88	2.2	4.89
Longer-term Concentration Used in Analysis (µg/L)	0.033	0.022	0.054

Other General Inputs: Application rate: 1 lb/acre, 1 application; Proportion of watershed treated: 1.0; Wetted in: No; Drift: None; Incorporation Depth: 0 cm.

[1] Appendix 2, Table 2-1.

[2] Appendix 2, Table 2-2.

[3] Central estimate and range from U.S. EPA/OPP/EFED 2012, Tables 2-2 and 3-1. Note that higher value for Koc is used to estimate lower bound concentration in water.

[4] U.S. EPA/OPP/EFED 2012, Table 3-1.

See Section 3.2. for discussion.

NOTE: The proportion of the treated watershed may be modified in the above table. The last two rows are fields. The values in the fields must be updated in the proportion of the treated watershed is changed. Place the cursor on each field, right click, and select "Update Field"

Table 5: Summary of toxicity values used in human health risk assessment

Acute Oral – Incidental Short term (1-30 days)

Element	Derivation of RfD
EPA Document	U.S. EPA/OPP/HED 2012, Table A.2.1, p. 29.
Study	Not specified in U.S. EPA/OPP/HED (2012) or U.S. EPA/OPP (1999a).
NOAEL Dose	41.3 mg/kg bw/day
LOAEL Dose	113 mg/kg bw/day
LOAEL Endpoint(s)	Kidney, minimal to slight hyperplasia of epithelium of proximal convoluted tubules.
Species, sex	Mice, NS
Uncertainty Factor/MOE	100
Equivalent RfD	0.413 mg/kg bw/day

Chronic Oral – lifetime exposure

Element	Derivation of RfD
EPA Document	U.S. EPA/OPP/HED 2012, Table A.2.1, p. 29; U.S. EPA/OPP 1999a, p. 21.
Study	MRID 41250502, rat chronic study, 23-29 months.
NOAEL Dose	2.0 mg/kg bw/day
LOAEL Dose	4.0 mg/kg bw/day
LOAEL Endpoint(s)	Kidney, epithelial hyperplasia in the renal proximal convoluted tubules of female rats.
Species, sex	Rats, females
Uncertainty Factor	100
Chronic RfD	0.02 mg/kg bw/day

Inhalation Exposures

Element	Derivation of RfD
EPA Document	U.S. EPA/OPP/HED 2012, Table A2.1, p. 29
Study	Not specified in U.S. EPA/OPP/HED (2012) or U.S. EPA/OPP (1999a).
NOAEL Dose	None specified
LOAEL Dose	0.002 mg/L
LOAEL Endpoint(s)	Hypoactivity, gasping, lacrimation, nasal discharge, piloerection, ptosis (eyelid droop), and respiratory gurgle.
Species, sex	Rats, M/F
Uncertainty Factor for Acute	100
Human Equivalent Dose	0.0004 mg/L or 400,000 ng/m^3
Equivalent Acute RfC	0.000004 mg/L or 4,000 ng/m^3
Human Equivalent Dose	0.00006 mg/L or 60,000 ng/m^3
MOE for Longer-term	1000
Equivalent Intermediate-term RfC	0.00000006 mg/L or 60 ng/m^3

See Section 3.3 for discussion.

Table 6: Summary of toxicity values used in ERA

Group/Duration	Organism	Endpoint	Toxicity Value (a.i.)	Reference
Terrestrial Animals				
Acute				
Mammals (including canids)		Adjusted Acute NOAEL	34.3 mg/kg bw	Section 4.3.1.1.1
Birds		Adjusted Acute NOAEL	530 mg/kg bw	Section 4.3.1.2.1
Honey Bee (contact)		Marginal NOAEL	1560 mg/kg bw	Section 4.3.1.3.1
Longer-term				
Mammals		Chronic NOAEL	2 mg/kg bw/day	Section 4.3.1.1.2
Bird		Adjusted chronic NOAEL	6.5 mg/kg bw/day	Section 4.3.1.2.2
Aquatic Animals				
Acute				
Fish	Sensitive	Trout LC50 of 10 µg/L ÷ 20	0.0005 mg/L	Section 4.3.2.1
	Tolerant	Tilapia LC_{50} of 120 µg/L ÷ 20	0.006 mg/L	Section 4.3.2.1
Invertebrates	Sensitive	Daphnid LC_{50} ÷ 20	0.0027 mg/L	Section 4.3.3.3.1
	Tolerant	Mussel EC_{50} ÷ 20	0.014 mg/L	Section 4.3.3.3.2
Longer-term				
Fish	Sensitive	Not identified.	N/A	Section 4.3.2.1.2
	Tolerant	Use chronic value	0.0013 mg/L	Section 4.3.2.1.2
Invertebrates	Sensitive	Daphnid NOAEC	0.0006 mg /L	Section 4.3.3.3.1
	Tolerant	No data	N/A	Section 4.3.2.3.2.
Aquatic Plants				
Algae	Sensitive	NOAEC, diatom	0.0039 mg/L	Section 4.3.2.4.1.1
	Tolerant	NOAEC, green algae	0.050 mg/L	Section 4.3.2.4.1.2
Macrophytes	Sensitive			Section 4.3.3.4
	Tolerant			Section 4.3.3.4

Appendix 1: FIRST Runs

Central Estimate

```
    RUN No.   1 FOR Chlorothalonil   ON   None          * INPUT VALUES *
   ---------------------------------------------------------------------
    RATE (#/AC)   No.APPS &   SOIL  SOLUBIL  APPL TYPE  %CROPPED INCORP
     ONE(MULT)    INTERVAL    Koc   (PPB )   (%DRIFT)     AREA    (IN)
   ---------------------------------------------------------------------
  1.000(  1.000)   1   1    4040.0  800.0   GRANUL( 0.0) 100.0   0.0


   FIELD AND RESERVOIR HALFLIFE VALUES (DAYS)
   ---------------------------------------------------------------------
   METABOLIC  DAYS UNTIL  HYDROLYSIS   PHOTOLYSIS   METABOLIC  COMBINED
    (FIELD)  RAIN/RUNOFF  (RESERVOIR)  (RES.-EFF)   (RESER.)   (RESER.)
   ---------------------------------------------------------------------
     11.20        2           0.00    0.40-   49.60    0.88       0.86


   UNTREATED WATER CONC (MICROGRAMS/LITER (PPB)) Ver 1.1.1  MAR 26, 2008
   ---------------------------------------------------------------------
        PEAK DAY  (ACUTE)      ANNUAL AVERAGE (CHRONIC)
          CONCENTRATION            CONCENTRATION
   ---------------------------------------------------------------------
             20.597                     0.237
```

Lower Bound

```
    RUN No.   2 FOR Chlorothalonil   ON   None          * INPUT VALUES *
   ---------------------------------------------------------------------
    RATE (#/AC)   No.APPS &   SOIL  SOLUBIL  APPL TYPE  %CROPPED INCORP
     ONE(MULT)    INTERVAL    Koc   (PPB )   (%DRIFT)     AREA    (IN)
   ---------------------------------------------------------------------
  1.000(  1.000)   1   1   11935.0  800.0   GRANUL( 0.0) 100.0   0.0


   FIELD AND RESERVOIR HALFLIFE VALUES (DAYS)
   ---------------------------------------------------------------------
   METABOLIC  DAYS UNTIL  HYDROLYSIS   PHOTOLYSIS   METABOLIC  COMBINED
    (FIELD)  RAIN/RUNOFF  (RESERVOIR)  (RES.-EFF)   (RESER.)   (RESER.)
   ---------------------------------------------------------------------
      5.76        2           0.00    0.40-   49.60    0.29       0.29


   UNTREATED WATER CONC (MICROGRAMS/LITER (PPB)) Ver 1.1.1  MAR 26, 2008
   ---------------------------------------------------------------------
        PEAK DAY  (ACUTE)      ANNUAL AVERAGE (CHRONIC)
          CONCENTRATION            CONCENTRATION
   ---------------------------------------------------------------------
             15.685                     0.156
```

Upper Bound

```
RUN No.   3 FOR chlorothalonil   ON   None          * INPUT VALUES *
   ---------------------------------------------------------------------
    RATE (#/AC)   No.APPS &   SOIL  SOLUBIL  APPL TYPE  %CROPPED INCORP
     ONE(MULT)    INTERVAL    Koc   (PPB )   (%DRIFT)     AREA    (IN)
   ---------------------------------------------------------------------
  1.000(  1.000)   1   1    1121.0  800.0   GRANUL( 0.0) 100.0   0.0


   FIELD AND RESERVOIR HALFLIFE VALUES (DAYS)
   ---------------------------------------------------------------------
   METABOLIC  DAYS UNTIL  HYDROLYSIS   PHOTOLYSIS   METABOLIC  COMBINED
    (FIELD)  RAIN/RUNOFF  (RESERVOIR)  (RES.-EFF)   (RESER.)   (RESER.)
   ---------------------------------------------------------------------
     16.64        2           0.00    0.40-   49.60    1.47       1.43


   UNTREATED WATER CONC (MICROGRAMS/LITER (PPB)) Ver 1.1.1  MAR 26, 2008
   ---------------------------------------------------------------------
        PEAK DAY  (ACUTE)      ANNUAL AVERAGE (CHRONIC)
          CONCENTRATION            CONCENTRATION
   ---------------------------------------------------------------------
             34.869                     0.383
```

Appendix 2: Check of EPA Calculations

Table A2-1: Aerobic soil metabolism 80% Confidence Interval for 90% upper bound

Item Number	Value	Square of Error
1	57	2097.640000
2	22	116.640000
3	18	46.240000
4	15	14.440000
5	14	7.840000
6	10	1.440000
7	10	1.440000
8	5	38.440000
9	2	84.640000
10	1	104.040000
11	1	104.040000
12	1	104.040000
13	0.5	114.490000
14	0.3	118.810000
Average	11.200000	
SSE	2954.180000	
Sample Standard Deviation	15.074635	
Critical Value of t at 0.1	1.350	
Value of 5% Lower Bound	5.7610313	
Value of 95% Upper Bound	16.6389687	

Note: In U.S. EPA/OPP/EFED (2012, Table 3-2, p. 107), an initial value of 87 is listed. This appears to be an error. Deleting this value is consistent with the EPA calculations as well as the summary in U.S. EPA/OPP/EFED 2012, Table 2-2. Note also that an n of 14 would typically call for a t-value of 1.350 rather than the value of 1.282 (which is the approximation for an infinitely high n). The correct t-value of 1.35 is used above.

Table A2-2: Aerobic aquatic metabolism 80% Confidence Interval for 90% upper bound

Item Number	Value	Square of Error
1	2.6	2.946946
2	1.4	0.266945
3	0.8	0.006944
4	0.3	0.340277
5	0.1	0.613611
6	0.1	0.613611
Average	0.883333	
SSE	4.788334	
Sample Standard Deviation	0.978605	
Critical Value of t at 0.1	1.476	
Value of 5% Lower Bound	0.2936506	
Value of 95% Upper Bound	1.4730154	

The above is consistent with the calculations in U.S. EPA/OPP/EFED 2012, Table 3-2, p. 108.