

**SRR-CWDA-2011-00106**  
**Revision 0**

**Qualification and Management of  $K_d$  Data for  
Use in C&WDA Performance Assessments**

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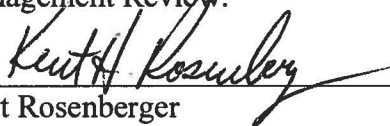


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### ACRONYMS/ABBREVIATIONS

C&WDA	Closure and Waste Disposal Authority
EPA	Environmental Protection Agency
$K_d$	Partition or Distribution Coefficient, parameter used in transport calculations
LUT	Lookup Table
NRC	U.S. Nuclear Regulatory Commission
PA	Performance Assessment
QA	Quality Assurance
RAI	Request for Additional Information
SME	Subject Matter Expert

## 1.0 INTRODUCTION

The Savannah River Site's Closure and Waste Disposal Authority (C&WDA) is responsible for developing Liquid Waste Performance Assessment (PA) models to support various regulatory documents. PA models are complex simulations that rely on many input parameters to appropriately estimate the potential migration of contaminants. According to the U.S. Environmental Protection Agency (EPA), the input "parameter known as the partition (or distribution) coefficient ( $K_d$ ) is one of the most important parameters used in estimating the migration potential of contaminants present in aqueous solutions in contact with surface, subsurface and suspended solids." [EPA 402-R-99-004A]

The EPA explains the significance of this parameter as follows:

"As typically used in fate and contaminant transport calculations, the  $K_d$  is defined as the ratio of the contaminant concentration associated with the solid to the contaminant concentration in the surrounding aqueous solution when the system is at equilibrium. Soil and geochemists knowledgeable of sorption processes in natural environments have long known that generic or default  $K_d$  values can result in significant error when used to predict the absolute impacts of contaminant migration or site-remediation options. Therefore, for site-specific calculations,  $K_d$  values measured at site-specific conditions are absolutely essential." [EPA 402-R-99-004A]

### 1.1 Purpose

The study of this chemical property, with respect to transport through various media, is a dynamic field in which new research frequently improves existing data. As new studies or literature reviews are completed, subject matter experts (SMEs) assimilate the data and document their findings in technical reports. This document provides a path forward to effectively manage these updates to site-specific  $K_d$  values for use in PAs. Effective management of this data must meet two requirements:

1. The process must be dynamic; and
2. The integrity of the data must be ensured.

These two requirements are discussed further below. By applying this approach, this document may be used as a single reference document for all PA  $K_d$  values and provides a single source to verify all  $K_d$  values against during PA model qualification.

#### 1.1.1 Dynamic Process

The process must be dynamic. PA results are known to be sensitive to  $K_d$  values; therefore, it is important to ensure that the most current  $K_d$  values available are captured for use in the development of PAs. This process shall provide a streamlined approach that allows for frequent updating without creating an unnecessary burden on configuration management or quality assurance practices.

#### 1.1.2 Ensuring Data Integrity

The integrity of the data must be ensured. Despite the first requirement, successful development of PA models is contingent upon the pedigree of data used as inputs; therefore

this process must include provisions to verify, and document, that the data is of a quality that is appropriate for use in PAs.

## **1.2 Scope**

This document summarizes K<sub>d</sub> data from approved technical reports prepared by SMEs and documents which values were applied to various PAs. Such data is already qualified for PA use. However, the instructions provided herein provide confidence that the data gathered into the data repository of C&WDA PA K<sub>d</sub> values meet the requirements for data qualification and data management as described in the E7 Manual, Procedure 3.70: *Qualification of Existing Data* and Procedure 5.80: *Data Management*.

## 2.0 DATA MANAGEMENT PROCESS

The streamlined approach for managing updates to K<sub>d</sub> values shall leverage existing tools, as used by C&WDA. Specifically, data shall be maintained within an MS Excel file and the MS Excel file shall be stored in the LWO Document Library. As SMEs complete technical reports, C&WDA shall review the K<sub>d</sub> values and update the MS Excel file to reflect the most current values available, as appropriate for use in PAs.

The following sections shall describe the data within the MS Excel file and instructions for updating and storing data.

### 2.1 Data Description

The MS Excel filename is “CWDA\_PA\_Kd\_LUT\_MMDDYYYY.xls” –

“CWDA” identifies the organization with ownership of this data (C&WDA).

“PA” identifies that this data is for use in Performance Assessments.

“Kd” indicates that this file contains K<sub>d</sub> values.

“LUT” indicates that the data in the file is structured as a lookup table.

“MMDDYYYY” is a variable to indicate the date of the most recent update to the file, where:

MM indicates the month (01 to 12);

DD indicates the day (01 thru 31); and

YYYY indicates the year.

#### 2.1.1 Sheet: ReadMe

The Sheet: “ReadMe” provides general user instructions for C&WDA. These instructions are provided to ensure that this data is appropriately used and that the integrity of the data is maintained (see Section 3.0 for more information). This sheet also provides a complete record of data qualification as described in Section 3.

#### 2.1.2 Sheet: Refs

The Sheet: “Refs” provides a complete listing of the references for the data found within the MS Excel file. The references are formatted for use in C&WDA documents (i.e., the references may be copied and pasted into a C&WDA document reference list with minimal formatting changes).

#### 2.1.3 Sheet: Kd

The Sheet: “Kd” provides (1) the most current K<sub>d</sub> values available for PA development and (2) the K<sub>d</sub> data sets used in previous C&WDA PAs. In addition to the K<sub>d</sub>s, the source document for each value is also provided. For illustrative purposes, Figure 2.1-1 provides a screen capture from this sheet and is discussed below.

Figure 2.1-1: Screen Capture from CWDA\_PA\_Kd\_LUT\_MMDDYYYY.xls, Sheet: Kds

Element	Material	Kd	Uni	Associated PA	PA Document ID	PA R	Location in PA	Cement Ty	Reference	Location in Reference	Reference Date	Data Typ	Notes
Ac	clayey	8500.0	mL/g	Current	NA	0	NA	NA	SRNL-STI-2009-00473	Table 16	3/15/2010	Analogue	Ce(III) data used as analogue.
Ac	oxidizing middl	6000.0	mL/g	Current	NA	0	NA	concrete	SRNL-STI-2009-00473	Table 17	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	oxidizing old	600.0	mL/g	Current	NA	0	NA	concrete	SRNL-STI-2009-00473	Table 17	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	oxidizing youn	6000.0	mL/g	Current	NA	0	NA	concrete	SRNL-STI-2009-00473	Table 17	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	reducing middl	7000.0	mL/g	Current	NA	0	NA	concrete	SRNL-STI-2009-00473	Table 18	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	reducing old	1000.0	mL/g	Current	NA	0	NA	concrete	SRNL-STI-2009-00473	Table 18	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	reducing youn	7000.0	mL/g	Current	NA	0	NA	concrete	SRNL-STI-2009-00473	Table 18	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	sandy	1100.0	mL/g	Current	NA	0	NA	NA	SRNL-STI-2009-00473	Table 16	3/15/2010	Analogue	Ce(III) data used as analogue.
Ac	waste	0	mL/g	Current	NA	0	NA	NA	Assigned a value of zero	NA	1/1/1900	NA	Value imposed for PORFLOW modeling purpo
Ac	clayey	8500.0	mL/g	FTF	SRS-REG-2007-00002	1	Table 4.2-29	NA	WSRC-TR-2006-00004	Table 10	2/28/2006	Analogue	Ce(III) data used as analogue.
Ac	oxidizing middl	5000.0	mL/g	FTF	SRS-REG-2007-00002	1	Table 4.2-33	concrete	WSRC-TR-2006-00004	Table 13	2/28/2006	Analogue	Am data used as analogue.
Ac	oxidizing old	500.0	mL/g	FTF	SRS-REG-2007-00002	1	Table 4.2-33	concrete	WSRC-TR-2006-00004	Table 13	2/28/2006	Analogue	Am data used as analogue.
Ac	oxidizing youn	5000.0	mL/g	FTF	SRS-REG-2007-00002	1	Table 4.2-33	concrete	WSRC-TR-2006-00004	Table 13	2/28/2006	Analogue	Am data used as analogue.
Ac	reducing middl	5000.0	mL/g	FTF	SRS-REG-2007-00002	1	Table 4.2-33	concrete	WSRC-TR-2006-00004	Table 14	2/28/2006	Analogue	Am data used as analogue.
Ac	reducing old	500.0	mL/g	FTF	SRS-REG-2007-00002	1	Table 4.2-33	concrete	WSRC-TR-2006-00004	Table 14	2/28/2006	Analogue	Am data used as analogue.
Ac	reducing youn	5000.0	mL/g	FTF	SRS-REG-2007-00002	1	Table 4.2-33	concrete	WSRC-TR-2006-00004	Table 14	2/28/2006	Analogue	Am data used as analogue.
Ac	sandy	1100.0	mL/g	FTF	SRS-REG-2007-00002	1	Table 4.2-29	NA	WSRC-TR-2006-00004	Table 10	2/28/2006	Analogue	Ce(III) data used as analogue.
Ac	clayey	8500.0	mL/g	HTF	SRR-CWDA-2010-00128	0	Table 4.2-29	NA	SRNL-STI-2009-00473	Table 16	3/15/2010	Analogue	Ce(III) data used as analogue.
Ac	oxidizing middl	6000.0	mL/g	HTF	SRR-CWDA-2010-00128	0	Table 4.2-33	concrete	SRNL-STI-2009-00473	Table 17	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	oxidizing old	600.0	mL/g	HTF	SRR-CWDA-2010-00128	0	Table 4.2-33	concrete	SRNL-STI-2009-00473	Table 17	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	oxidizing youn	6000.0	mL/g	HTF	SRR-CWDA-2010-00128	0	Table 4.2-33	concrete	SRNL-STI-2009-00473	Table 17	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	reducing middl	7000.0	mL/g	HTF	SRR-CWDA-2010-00128	0	Table 4.2-33	concrete	SRNL-STI-2009-00473	Table 18	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	reducing old	1000.0	mL/g	HTF	SRR-CWDA-2010-00128	0	Table 4.2-33	concrete	SRNL-STI-2009-00473	Table 18	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	reducing youn	7000.0	mL/g	HTF	SRR-CWDA-2010-00128	0	Table 4.2-33	concrete	SRNL-STI-2009-00473	Table 18	3/15/2010	Analogue	Am, Ce, Y values used as analogue.
Ac	sandy	1100.0	mL/g	HTF	SRR-CWDA-2010-00128	0	Table 4.2-29	NA	SRNL-STI-2009-00473	Table 16	3/15/2010	Analogue	Ce(III) data used as analogue.
Ac	clayey	8500.0	mL/g	SDF	SRR-CWDA-2009-00017	0	Table 4.2-15	NA	WSRC-TR-2006-00004	Table 10	2/28/2006	Analogue	Ce(III) data used as analogue.
Ac	oxidizing middl	6000.0	mL/g	SDF	SRR-CWDA-2009-00017	0	Table 4.2-18	concrete	WSRC-TR-2007-00640	Table 10	12/1/2007	Analogue	Am(III), Ce(III), Y(III) values used as analogue

**Note:** This image is provided for illustrative purposes only. Data presented in this image is not intended for qualified use. For current data, users must refer to the most current MS Excel file associated with this document, as described herein.



The column heading and description of the data are as follows:

- **Element** – Identifies the element by atomic symbol.
  - **Material** – Identifies the appropriate material or transport media that the K<sub>d</sub> values apply to. These include:
    - sandy - Sandy Soil (Vadose Zone)
    - clayey - Clayey Soil (Backfill)
    - oxidizing young - Oxidized Region I (Young Ox. Cement)
    - oxidizing middle - Oxidized Region II (Middle Ox. Cement)
    - oxidizing old - Oxidized Region III (Old Ox. Cement)
    - reducing young - Reduced Region I (Young Re. Cement)
    - reducing middle - Reduced Region II (Middle Re. Cement)
    - reducing old - Reduced Region III (Old Re. Cement)
    - waste - Zero K<sub>d</sub> value used for modeling purposes
  - **K<sub>d</sub>** – K<sub>d</sub> value.
  - **Units** – The units assigned to the K<sub>d</sub> value. Generally mL/g is used.
  - **Associated\_PA** – A short identifier associated with specific C&WDA PAs, where:
    - **FTF** = F-Area Tank Farm,
    - **HTF** = H-Area Tank Farm,
    - **SDF** = Saltstone Disposal Facility, and
    - **Current** = the most current data available (for use in future PAs).
- Note:** For future use, new identifiers may be incorporated. For example, in response to SDF Requests for Additional Information (RAIs) from the U.S. Nuclear Regulatory Commission (NRC), an Alternative Sensitivity Case K is currently under development. The K<sub>d</sub> values for this sensitivity case will likely be archived within CWDA\_PA\_K<sub>d</sub>\_LUT\_MMDDYYYY.xls as “SDF\_K” or “SDF\_PA-8”.
- **PA\_Document\_ID** and **PA\_Rev** – The document identifier and revision number for the associated PA report. For the “Current” dataset, the document is “NA”. The default PA revision number is zero.
  - **Location\_in\_PA** – Documented traceability, describes where to find the K<sub>d</sub> value within the respective PA document. PA documents are fully cited in the Sheet: “Refs”.
  - **CementType** – Used to identify if cementitious values are intended to be applied specifically to saltstone grout or concrete material. The default entry “NA” indicates that this field does not apply to the K<sub>d</sub>.
  - **Reference** – Document identifier for the source document.

- **Location\_in\_Reference** – Documented traceability, describes where to find the  $K_d$  value within the source document. Reference documents are fully cited in the Sheet: “Refs”.
- **Reference Date** – Approval date for the source document. For  $K_d$ s with assumed zero values, the date of the associated PA document is applied. To normalize data entries, all “N/A” reference entries are assigned a default date of 1/1/1900.
- **DataType** – Defines the type of source, where:
  - **“Site Data”** indicates that the  $K_d$  value is based upon site-specific studies,
  - **“Literature”** indicates that the value was determined based upon an evaluation of literature values,
  - **“Analogue”** indicates that the value used is an analogue value based upon the  $K_d$  of a similar element,
  - **“Undetermined”** indicates that the data type could not be determined based upon the information provided within the source document.
  - **“NA”** indicates that the element was not used within the respective PA; therefore, the data type is non-applicable.
  - **“Zero Value”** indicates that, in the absence of more sufficient data, a conservative value of zero was assumed for use in the associated PA.
- **Saltstone** – Column is used to discern between cementitious/grout  $K_d$  values that are specific to saltstone grout modeling (i.e., 45% slag) and other cementitious/grout  $K_d$  values, where:
  - **“NA”** indicates that the material is not a cementitious/grout material, therefore, this information does not apply for this material property. “NA” applies to sandy, clayey, and waste materials.
  - **“No”** indicates that the value is not specific to saltstone grout.
  - **“Yes”** indicates that the data, if used in previous PAs, was used as a  $K_d$  value for saltstone or saltstone equivalent material. If the value is applied to a “Current” element, the value is only to be applied to saltstone-specific grout. If there is no “Yes” entry for a specific radionuclide, it is appropriate to default to the non-saltstone specific cementitious  $K_d$  value.
- **Notes** – Provides additional supporting information.

The data in this file is subject to change, as needed to support future PA work. Users of this data shall be responsible for updating this qualification and data management report as deemed appropriate.

## 2.2 File Management and Data Updates

MS Excel was selected for this application as it is the most accessible data tool available to C&WDA.

Updates to data may be accomplished by performing the following steps:

- 1) Access the LWO Document Library and find the entry for this document (SRR-CWDA-2011-00106).
- 2) The document entry will have MS Excel files within the “Supporting Files” field. Each file shall be named, as described above, according to the date of the last file change or data modification. Based upon the dates provided in the filenames, identify the most current MS Excel file.
- 3) Right click on the file and save it to a working directory (e.g., your desktop or department server).
- 4) Make changes to the data or file. If the changes impact this document, revise this document as needed.
- 5) Within the ReadMe sheet, under “Change History”, provide a summary description of what changed, relative to the previous version of the file. You **MUST** enter a Quality Assurance (QA) status of “N” for non-qualified to indicate that the changes have not been checked.
- 6) Ask another C&WDA staff member to check your work and document their checking, according to the instructions provided in Section 3.
- 7) Save the updated/checked file with a new name according to the naming convention provided in Section 2.1.
- 8) Post the new updated/checked file to the “Supporting Files” field of LWO Document Library entry for this document.

### 3.0 DATA QUALIFICATION PROCESS

The MS Excel file: CWDA\_PA\_Kd\_LUT\_MMDDYYYY.xls serves as the K<sub>d</sub> data repository for C&WDA PAs. This file does not contain any newly developed data, calculations, or test results. Rather the file acts a repository of already existing data. This repository facilitates quick access to the data and allows effective data analysis. All of the information comes from approved technical reports and is qualified for use in C&WDA PAs. The data qualification process provided here has been developed to ensure that data is properly captured and to identify and correct potential data entry errors.

#### 3.1 Data Verification

Any changes to the K<sub>d</sub> data within the MS Excel file must be independently verified. To verify, a checker should compare changed data against the source data found in the appropriate technical report. Any errors must be resolved before the data can be used for qualified work. Once the checker and the originator are both satisfied that the data in the MS Excel file reflect the source data, the checker must document the QA status of the data (see Section 3.2).

#### 3.2 QA Documentation

QA status should be documented upon completion of data verification.

Within the MS Excel file, open the sheet: ReadMe. In the row immediately following the last Change History entry, enter the date and indicate “Data verified by [insert name of checker]”. Then enter a QA status of “QA”. Return the file to the originator to complete Steps 7 and 8 of Section 2.2.

## 4.0 REFERENCES

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**Note:** References to specific K<sub>d</sub> values are captured within the MS Excel file that accompanies this report, as discussed in Section 2.1.2.

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E7 Manual, Procedure 3.70, *Conduct of Engineering and Technical Support Procedure Manual, Qualification of Existing Data*, Savannah River Site, Aiken, SC, Rev. 4.

E7 Manual, Procedure 5.80, *Conduct of Engineering and Technical Support Procedure Manual, Data Management*, Savannah River Site, Aiken, SC, Rev. 4.

EPA-402-R-9-004A, *Understanding Variation in Partition Coefficient, K<sub>d</sub> Values: Volume I: The K<sub>d</sub> Model, Methods of Measurement, and Application of Chemical Reaction Codes*, U.S. Environmental Protection Agency, Washington, DC, August 1999.