Revising the EPA Dilution-Attenuation Soil Screening Model for PFAS

Mark L. Brusseau[1,2,*] and Bo Guo[2]

[1]Environmental Science Department and [2]Hydrology and Atmospheric Sciences Department

The University of Arizona

Tucson, AZ 85721

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[*]Corresponding author, Brusseau@arizona.edu

1   **Abstract**

2   Per and polyfluoroalkyl substances (PFAS) have been shown to be ubiquitous in the

3   environment, and one issue of critical concern is the leaching of PFAS from soil to groundwater.

4   The risk posed by contaminants present in soil is often assessed in terms of the anticipated impact

5   to groundwater through the determination of soil screening levels (SSLs). The U.S. Environmental

6   Protection Agency (EPA) established a soil screening model for determining SSLs. However, the

7   model does not consider the unique retention properties of PFAS and, consequently, the SSLs

8   established with the model may not represent the actual levels that are protective of groundwater

9   quality. The objective of this work is to revise the standard EPA SSL model to reflect the unique

10   properties and associated retention behavior of PFAS. Specifically, the distribution parameter used

11   to convert soil porewater concentrations to soil concentrations is revised to account for adsorption

12   at the air-water interface. Example calculations conducted for PFOS and PFOA illustrate the

13   contrasting SSLs obtained with the revised and standard models. A comparison of distribution

14   parameters calculated for a series of PFAS of different chain length shows that the significance of

15   air-water interfacial adsorption can vary greatly as a function of the specific PFAS. Therefore, the

16   difference between SSLs calculated with the revised versus standard models will vary as a function

17   of the specific PFAS, with greater differences typically observed for longer-chain PFAS. It is

18   anticipated that this revised model will be useful for developing improved SSLs that can be used

19   to enhance site investigations and management for PFAS-impacted sites.

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21   **Keywords**: PFAS; leaching; transport and fate; soil contamination

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23 **Synopsis**: The widely used EPA SSL model is revised for PFAS applications to account for

24 adsorption at the air-water interface.

25

Introduction

26   **Introduction**

27   Recent meta-analyses of field investigations have determined that the vadose zone is a

28   primary reservoir of per and polyfluoroalkyl substances (PFAS) at many PFAS-impacted sites

29   (1,2). A primary concern for these sites is the leaching of PFAS through the vadose zone to

30   groundwater, and the subsequent impairment of groundwater quality and associated potential risks

31   to human health. The risk posed by contaminants present in the vadose zone is often assessed in

32   terms of the anticipated impact to groundwater. An initial assessment of this risk is typically

33   conducted by comparing measured soil concentrations to soil screening levels (SSLs) that are

34   established to be protective of groundwater quality. It is important to note that SSLs are not cleanup

35   standards (3).

36   The U.S. Environmental Protection Agency (EPA) established a soil screening guidance in

37   1996 as a means to develop SSLs (3,4). The SSL is defined as the concentration of contaminant in

38   soil that is determined to be protective of human exposure via a specified exposure pathway. For

39   example, the methodology for calculating SSLs for the migration-to-groundwater pathway was

40   developed to identify concentrations in soil that have the potential to contaminate groundwater.

41   SSLs are risk-based concentrations derived from equations combining exposure information with

42   EPA toxicity data. The exposure information refers to the exposure pathway selected for

43   assessment (such as migration to groundwater) and to the soil concentrations present at the site.

44   The toxicity data refers to the standard used to set the target concentration for the relevant medium,

45   such as a maximum contaminant level used to establish the target groundwater concentration for

46   the migration-to-groundwater pathway.

47   The primary purpose of the EPA SSL approach is to conserve resources by identifying and

48   targeting the sites that pose the greatest concern and therefore warrant further investigation. It is

49   designed for use during the early stages of site investigations, when there is typically limited

50   information about subsurface properties and conditions. The SSL guidance was developed

51   specifically for application at Comprehensive Environmental Response, Compensation, and

52   Liability Act (CERCLA) national priorities list (Superfund) sites. However, the EPA SSL

53   guidance has been widely used for a diversity of sites and applications. It is the standard approach

54   for developing SSLs for sites with soil contamination.

55   The magnitudes of leaching and mass discharge to groundwater are governed by the

56   concentration of contaminant in soil porewater and the infiltration/recharge rate. The porewater

57   concentration in turn is mediated by multiple processes that affect the retention, attenuation, and

58   leaching of the contaminant in the vadose zone. The EPA SSL guidance is based on a simple

59   dilution-attenuation (DAF) mass-balance model. As for any screening model, the EPA DAF model

60   is based on a suite of simplifying assumptions. These include the assumption that retention of the

61   contaminant occurs solely by sorption to the soil solids and partitioning into the soil atmosphere,

62   and that sorption is linear, instantaneous (under equilibrium conditions), and associated only with

63   the organic-carbon component of the soil. The SSL guidance was established for application to

64   standard Superfund contaminants such as metals, chlorinated-solvent compounds, and

65   hydrocarbon-fuel constituents. Hence, the model does not consider the unique retention properties

66   of PFAS and, consequently, the SSLs established with the method may not represent the actual

67   levels that are protective of groundwater quality.

68   Field investigations, mathematical modeling, and bench-scale transport studies have

69   demonstrated that PFAS retention and transport in the vadose zone is typically more complex than

70   other types of contaminants such as chlorinated-solvent compounds and hydrocarbon-fuel

71   constituents. Specifically, as surfactants, PFAS adsorb at air-water interfaces in soils, which can

72   provide a source of significant retention in some cases (5-19). The magnitude of retention by air-

73   water interfacial adsorption depends upon several factors, including PFAS structure and

74   concentration, soil properties, solution chemistry, and the presence of co-solutes (5,6,9,11-13,17-

75   18,20-27). Sorption by the solid phase (soil particles) is another process of significance for PFAS.

76   Due to their molecular properties, PFAS sorption is often more complex compared to other

77   contaminants in that multiple soil constituents and associated mechanisms may be involved (28-

78   33). As a result of air-water interfacial adsorption and multi-mechanism sorption, the retention of

79   PFAS in the vadose zone can be significantly greater compared to traditional organic

80   contaminants. Therefore, efforts to characterize the distribution or transport of PFAS in the vadose

81   zone, including the determination of representative SSLs, should consider the unique properties of

82   PFAS.

83   The objective of this work is to revise the standard EPA SSL guidance to reflect the unique

84   properties and associated retention behavior of PFAS. The development of the standard EPA DAF

85   model is first presented, along with the accompanying assumptions. This model is then revised by

86   incorporating a term for air-water interfacial adsorption into the distribution parameter used to

87   convert soil porewater concentrations to soil concentrations. Example calculations are conducted

88   to illustrate the contrasting results obtained with the revised and standard models. The additional

89   input parameters required for the revised model are discussed.

90

91   **METHODS**

92   **The Standard EPA DAF SSL Model**

93   The present work is focused on SSLs developed specifically for the migration-to-

94   groundwater pathway. The conceptual basis of this specific approach is discussed in Section 1 in

95 the Supplemental Information (SI) file. The basic procedure to determine SSLs starts with the

96 identification of a relevant target concentration for groundwater (i.e., saturated-zone porewater)

97 that is determined to be protective of groundwater quality. This target concentration is then

98 multiplied by the DAF to obtain the corresponding target leachate or soil porewater concentration

99 in the vadose zone. This step accounts for relevant dilution and attenuation of contaminant

100 concentrations during migration through the vadose zone to the receptor well. This soil porewater

101 concentration is then multiplied by a distribution term to calculate the corresponding soil

102 concentration. This latter step is conducted for two reasons. First, soil porewater concentrations

103 are rarely directly measured at field sites, whereas soil concentrations are the standard for vadose-

104 zone characterization and are routinely measured. Second, most contaminants of concern are

105 present in additional phases in a soil sample beyond the aqueous phase (porewater), such as sorbed

106 by the solids, and thus total concentrations in the soil are typically greater than porewater

107 concentrations. It is observed that the procedure involves a set of backward-moving calculations

108 starting with the target groundwater concentration and progressing to the SSL.

109   There are two key parameters of the DAF model, the DAF term and the distribution term.

110 The DAF comprises the product of two components, the dilution factor (DF) and the attenuation

111 factor (AF), i.e., DAF = DF × AF. The EPA soil screening guidance addresses only one of these

112 dilution-attenuation processes, specifically contaminant dilution in groundwater. The DF is

113 determined by a simple mixing-zone equation derived from a water-balance relationship that

114 compares the rates of infiltration/recharge and groundwater flow. Detailed discussion of this term

115 is presented in the original EPA documents (3,4). The default value set by the EPA is 20. It is

116 critical to note that the standard EPA SSL model does not account for attenuation during transport

117 in the vadose zone or groundwater. Hence, the AF is set by default to 1, and the default DAF is

118 20. It is also important to recognize that the default assumption of AF = 1 is the most conservative

119 approach possible in terms of accounting for the impacts of attenuation processes on leaching in

120 the vadose zone. Namely, this approach assumes that there is no attenuation and, therefore, that

121 leaching rates of the contaminant are equivalent to those of a nonreactive (conservative) solute.

122   The distribution term is developed from a standard mass balance of contaminant

123 distribution in a soil volume sample. The complete development is given in the SI file (Section 2

124 in SI), along with underlying assumptions (Section 3 in SI). The EPA DAF SSL model is given as

125 (3,4):

126 $$SSL = C_{soil} = C_{gw}DAF[K_d + (\theta_w + \theta_a H)\frac{1}{\rho_b}] \qquad [1]$$

127 where C_{gw} is the target groundwater concentration deemed to be protective of groundwater quality,

128 $C_{pw} = C_{gw} DAF$, K_d (L^3/M) is the sorption coefficient, H (-) is Henry's law constant, ρ_b is porous-

129 medium bulk density (M/L^3), θ_a is volumetric air content (L^3/L^3), and θ_w is volumetric water

130 content (L^3/L^3). Note that the soil concentration determined from this calculation is the SSL.

131   The standard EPA DAF model accounts for contaminant specificity through the

132 magnitudes of K_d and H in the distribution term. The larger the term in brackets in equation (1),

133 the larger the SSL will be for a given target groundwater concentration. AF values may also vary

134 as a function of the contaminant, with for example larger resultant DAF values producing larger

135 SSLs. However, with the default setting of AF = 1, the DAF is independent of the contaminant

136 and solely a function of hydraulic (dilution) factors.

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138 **Development of the Revised DAF SSL Model**

139   The standard DAF model is revised to account for adsorption of PFAS at the air-water

140 interface. It is critical to note that this revision is directed to only the distribution term, which

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141 converts the calculated target soil porewater concentration to a corresponding soil concentration.

142 Hence, the revision accounts for the additional mass present in a soil sample that is adsorbed at the

143 air-water interface, the representation of which is critical to produce an accurate porewater-to-soil

144 conversion for PFAS. The revision does not account for the potential impact of air-water interfacial

145 adsorption on retention and associated attenuation during transport through the vadose zone. As

146 noted above, the default assumption for the standard DAF model is that there is no attenuation in

147 the vadose zone. Therefore, this revision does not impact the AF or DAF.

148　　　　Brusseau and colleagues have developed comprehensive retention models for the

149 distribution of PFAS in the vadose zone (6,16,34). The complete nondimensional distribution term,

150 R_d^{comp}, is given as (16):

151 $$R_d^{comp} = \left(1 + K_{d*}\frac{\rho_b}{\theta_w} + H\frac{\theta_a}{\theta_w} + K_n\frac{\theta_n}{\theta_w} + K_{aw*}\frac{a_{aw}}{\theta_w} + K_{nw*}\frac{a_{nw}}{\theta_w} + K_{an*}\frac{a_{an}}{\theta_w} + K_{c*}X_c\right) \quad [2]$$

152 where a_{an} is the specific air-NAPL interfacial area (L^2/L^3), a_{aw} is the specific air-water interfacial

153 area (L^2/L^3), a_{nw} is the specific NAPL-water interfacial area (L^2/L^3), K_{an*} is the nonlinear air-NAPL

154 interfacial adsorption coefficient (L^3/L^2), K_{aw*} is the nonlinear air-water interfacial adsorption

155 coefficient (L^3/L^2), K_{c*} is the nonlinear distribution coefficient for sorption by colloids (L^3/M), K_{d*}

156 is the nonlinear solid-phase adsorption coefficient (L^3/M), K_n is the NAPL-water partition

157 coefficient (-), K_{nw*} is the nonlinear NAPL-water interfacial adsorption coefficient (L^3/L^2), X_c is

158 the concentration of colloidal material in porewater (M/L^3) and θ_n is volumetric NAPL content

159 (L^3/L^3).

160　　　　Equation (2) accounts for the contributions of all potential relevant phases and domains

161 within a soil sample volume, with the exception of supramolecular structures such as micelles that

162 may exist as a separate phase. The R_d^{comp} term would be used to convert soil porewater

163 concentrations to soil concentrations by accounting for the presence of PFAS in all relevant

164 retention domains. Equation (2) can be modified on a site-specific basis by employing only those

165 terms that are relevant for that site. In the present work, it will be assumed that adsorption at the

166 air-water interface is the only additional source of retention beyond that of solid-phase sorption

167 and partitioning to soil atmosphere. The modified distribution term for this case is given by:

168 $$R_d^{Rev} = \left(1 + K_d \frac{\rho_b}{\theta_w} + H \frac{\theta_a}{\theta_w} + K_{aw} \frac{a_{aw}}{\theta_w}\right) \qquad [3]$$

169 where the K_d and K_{aw} have been simplified by assuming linear adsorption. Methods to account for

170 nonlinear adsorption are discussed by Brusseau and Guo (16). The revised SSL model in terms of

171 the nondimensional distribution factor format of Brusseau and Guo (16) is given by:

172 $$SSL^{Rev} = C_{gw} DAF \frac{\theta_w}{\rho_b} R_d^{Rev} \qquad [4]$$

173 The revised DAF SSL model presented in the original EPA format is given by:

174 $$SSL^{Rev} = C_{gw} DAF [K_d + (K_{aw} a_{aw} + \theta_w + \theta_a H) \frac{1}{\rho b}] \qquad [5]$$

175 Comparison of equations (1) and (5) reveals that the revised model differs from the original model

176 by the presence of the $K_{aw}a_{aw}$ term in the brackets, which accounts for contaminant that is adsorbed

177 at the air-water interface.

178

179 **RESULTS AND DISCUSSION**

180 **Illustrative Calculations of SSLs**

181 An illustrative application is presented to compare the differences in SSLs determined with

182 the revised and standard models due to the impact of air-water interfacial adsorption. A vadose

183 zone soil collected from a site in Tucson, AZ, is used as the representative porous medium.

184 Perfluorooctanesulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) are selected as the

185 representative PFAS. Values for the sorption coefficient, air-water interfacial adsorption

186 coefficient, and air-water interfacial area were obtained from prior studies (see references in Table

187 1). The input parameters used for the calculations are presented in Table 1, along with the SSLs

188 determined with the two models.

189   A SSL of 4.3 µg/kg is calculated for PFOS using the standard model. In comparison, a SSL

190 of 75.6 µg/kg is obtained with the revised model. The revised SSL is more than an order of

191 magnitude higher due to the impact of air-water interfacial adsorption. This difference could have

192 a significant impact on identification of sites or areas of sites of greatest concern. It is important

193 to recall that the revised SSL is based solely on correcting the distribution term used to convert

194 soil porewater concentration to soil concentration to account for the additional retention accrued

195 to air-water interfacial adsorption. Potential impacts of retention processes on PFAS leaching and

196 attenuation are not considered.

197

198 **Table 1**. Example Parameters and Calculated SSLs for PFOS and PFOA

Parameter	PFOS		PFOA	
	Standard Model	Revised Model	Standard Model	Revised Model
Dilution Factor (DF)	20	20	20	20
Attenuation Factor (AF)	1	1	1	1
Dilution-Attenuation Factor (DAF)	20	20	20	20
Bulk density (ρ_b, g/cm^3)	1.5	1.5	1.5	1.5
Water content (θ_w, -)	0.2	0.2	0.2	0.2
Air content (θ_a, -)	0.2	0.2	0.2	0.2
Porosity (n, -)	0.4	0.4	0.4	0.4
Sorption coefficient (K_d, cm^3/g)[a]	2	2	1	1
Henry's Law constant (H, -)	0	0	0	0
Air-water interfacial adsorption coefficient (K_{aw}, cm)[b]	NA	0.12	NA	0.008
Air-water interfacial area (a_{aw}, cm^{-1})[c]	NA	446	NA	446
Distribution term (R_d, -)	16	283.6	8.5	26.3
Target groundwater concentration (C_{gw}, µg/L)[d]	0.1	0.1	0.1	0.1
Soil Screening Level (SSL, µg/kg)	4.3	75.6	2.3	7.0

199   [a]Measured values from (12)
200   [b]Measured values from (22,24,25)
201   [c]Measured value from (8)

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204   The impact of contaminant properties on the SSL in the standard model was represented

205   through the values used for K_d and H in the distribution term. The air-water interfacial adsorption

206   coefficient employed in the revised model is also a function of the contaminant. Air-water

207   interfacial adsorption is a strong function of the molecular structure of the individual PFAS (20-

208   26). This is illustrated by comparing the SSLs determined for PFOA using all of the same

209   parameters as used for PFOS, with the exception of the sorption and air-water interfacial

210   adsorption coefficients (Table 1). The SSL determined for PFOA with the revised model is 7

211   µg/kg, compared to 75.6 µg/kg for PFOS. In addition, it is observed that the SSL calculated for

212   PFOA with the revised model is only a factor of three larger than the SSL calculated with the

213   standard model. Conversely, the two values differ by more than an order of magnitude for PFOS.

214   These results are due to the differential impact of air-water interfacial adsorption, wherein PFOS

215   has significantly greater interfacial activity compared to PFOA (as shown by their respective K_{aw}

216   values in Table 1).

217   The impact of chain length on the magnitude of air-water interfacial adsorption for a series

218   of PFAS is illustrated in Figure 1. The K_{aw} is observed to increase log-linearly with increasing

219   fluorinated-carbon chain length. More generally, K_{aw} is a log-linear function of the molar volume

220   (20,21,25). As a result, the significance of air-water interfacial adsorption can vary greatly as a

221   function of the specific PFAS. This means that the magnitude of the distribution term in equations

222   4 and 5 will vary as well. For example, as illustrated in Figure 1, the distribution factors for PFCAs

223   with <7 fluorinated carbons are close to 1 because of their comparatively small K_{aw} values.

224   Concomitantly, SSLs determined with the revised model for these PFAS will be similar to the

225   values determined with the standard model due to the minimal impact of air-water interfacial

226   adsorption. Therefore, the difference between SSLs calculated with the revised versus standard

227   models will vary as a function of the specific PFAS, with greater differences typically observed

228   for longer-chain PFAS.

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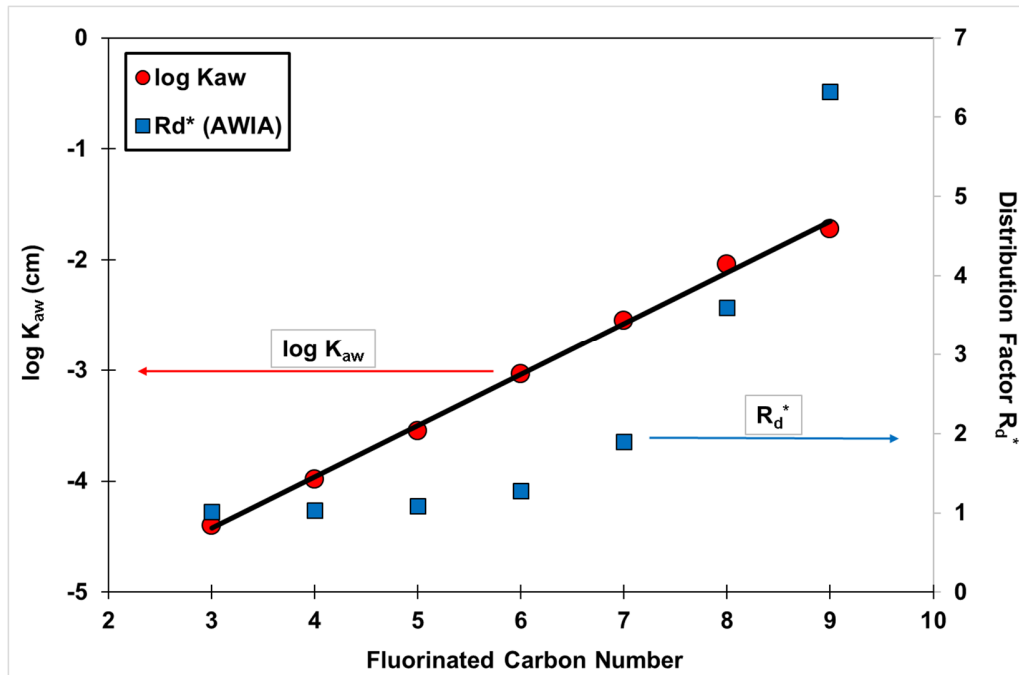
231 **Figure 1**. Correlation of air–water interfacial adsorption coefficient (K_{aw}) and distribution factor
232 R_d^* versus fluorinated carbon number for C4-C10 perfluorocarboxylic acids (PFCAs). The asterisk
233 denotes that this R_d accounts solely for air–water interfacial adsorption to illustrate specific
234 impacts. Measured data from transport experiments reported in Lyu et al. (17).
235

236   The revised model requires two additional input parameters, namely the air-water

237   interfacial adsorption coefficient and the air-water interfacial area. Measurement and estimation

238   of these parameters is discussed in the SI (Section 4), along with potential impacts of nonideal

239   processes. Also discussed in that section is the estimation of K_d.

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CONCLUSIONS

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244   There is currently great interest in determining SSLs for PFAS-impacted sites to protect

245   groundwater quality (e.g., 36-38). This issue is of great significance given the ubiquitous presence

246   of PFAS in soils across the globe. The standard EPA DAF model, which is the most widely used

247   method to establish SSLs, does not account for the unique properties of PFAS and how they may

248   impact retention and distribution in soil. This includes representing adsorption at air-water

249   interfaces, which can be a significant source of retention for many PFAS. The current model is

250   revised by incorporating a term for air-water interfacial adsorption into the distribution parameter

251   used to convert soil porewater concentrations to soil concentrations. Illustrative examples showed

252   that the SSLs determined for PFAS with the revised model may be significantly different from

253   those determined with the standard model. A comparison of distribution parameters calculated for

254   a series of PFAS of different chain length showed that the significance of air-water interfacial

255   adsorption can vary greatly as a function of the specific PFAS. Therefore, the difference between

256   SSLs calculated with the revised versus standard models will also vary as a function of the specific

257   PFAS, with greater differences typically observed for longer-chain PFAS. The specific PFAS for

258   which air-water interfacial adsorption would be comparatively insignificant will depend on site-

259   specific conditions.

260   It is critical to recognize that the model revision addresses only the distribution term that

261   serves to convert soil porewater concentrations to soil concentrations. The potential impact of air-

262   water interfacial adsorption, multi-mechanism sorption, and transformation processes on PFAS

263   leaching and attenuation in the vadose zone is not considered. This also means that potential factors

264   that can cause nonideal transport behavior (which may often manifest as enhanced rates of

265   leaching), such as heterogeneity and preferential flow, rate-limited mass-transfer processes, and

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266   the impact of PFAS mixtures and co-contaminants, are not considered. This is reflected in the use

267   of the standard EPA default assumption that there is no attenuation (AF = 1) in the vadose zone

268   (or groundwater) for the SSL calculations. This assumption is the most conservative approach

269   possible in terms of accounting for the impacts of retention and transformation processes on

270   leaching in the vadose zone. Namely, this approach assumes that there is no attenuation during

271   leaching and, therefore, that the leaching rates of the contaminant are equivalent to those of a

272   nonreactive (conservative) solute. Hence, this approach can be considered to account for the

273   potential impacts of nonideal transport behavior in the simplest manner possible by assuming that

274   there is no attenuation whatsoever. The influence of retention and transformation processes on

275   PFAS leaching can be accounted for by setting the AF to some value greater than 1. Or

276   alternatively, through the use of advanced mathematical models.

277   The revised model developed in the present work serves as a first step in determining more

278   robust SSLs that represent PFAS-specific retention and distribution behavior. It is anticipated that

279   this revised model will improve investigations and management for PFAS-impacted sites. The

280   limitations of the original EPA SSL model and by association the revised model are well

281   recognized. The original model was designed for use during the early stages of site investigations,

282   when there is typically limited information about subsurface properties and conditions (3,4). This

283   provision requires that the model be relatively simple and require a minimum of site-specific

284   information, while also being easily updatable when new information becomes available. The

285   model achieves these goals and has become an indispensable tool for site characterization and

286   management. However, there are certainly limitations to the effectiveness of the model. The EPA

287   guidance explicitly discusses options for when the model-associated assumptions are likely to be

288   invalid, noting specifically the option of using more sophisticated transport and fate models. Such

289 models are currently being developed specifically for PFAS. For example, an analytical-solution

290 based screening model has been published that accounts for several PFAS-specific transport and

291 fate processes (36). In addition, advanced numerical models have been developed to simulate

292 PFAS transport in the vadose zone (8,10,14,15,19). These models can accurately represent more

293 complex systems and conditions, but have greatly increased input-parameter requirements. We

294 believe that there is value in employing multiple modeling approaches, and that the simplest DAF

295 models serve an important role in site characterization that is complementary to the more advanced

296 models.

297

298 **ACKOWLEDGEMENTS**

303

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