



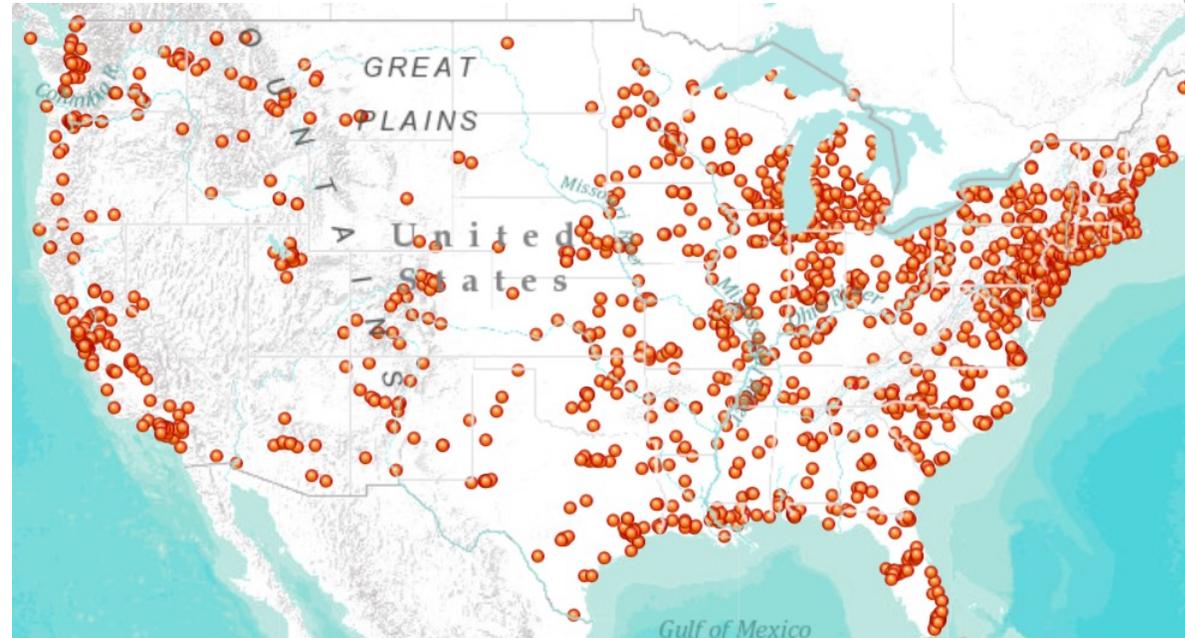
# Recommended Updates to the Soil-to-Groundwater Pathway in the U.S. EPA's 1996 Soil Screening Guidance

Seth Whiteaker and Alex Valdez

# Background

# Defining the Problem

- ▶ Groundwater pollution via soil contamination
- ▶ National Priorities List
- ▶ Need for effective risk characterization

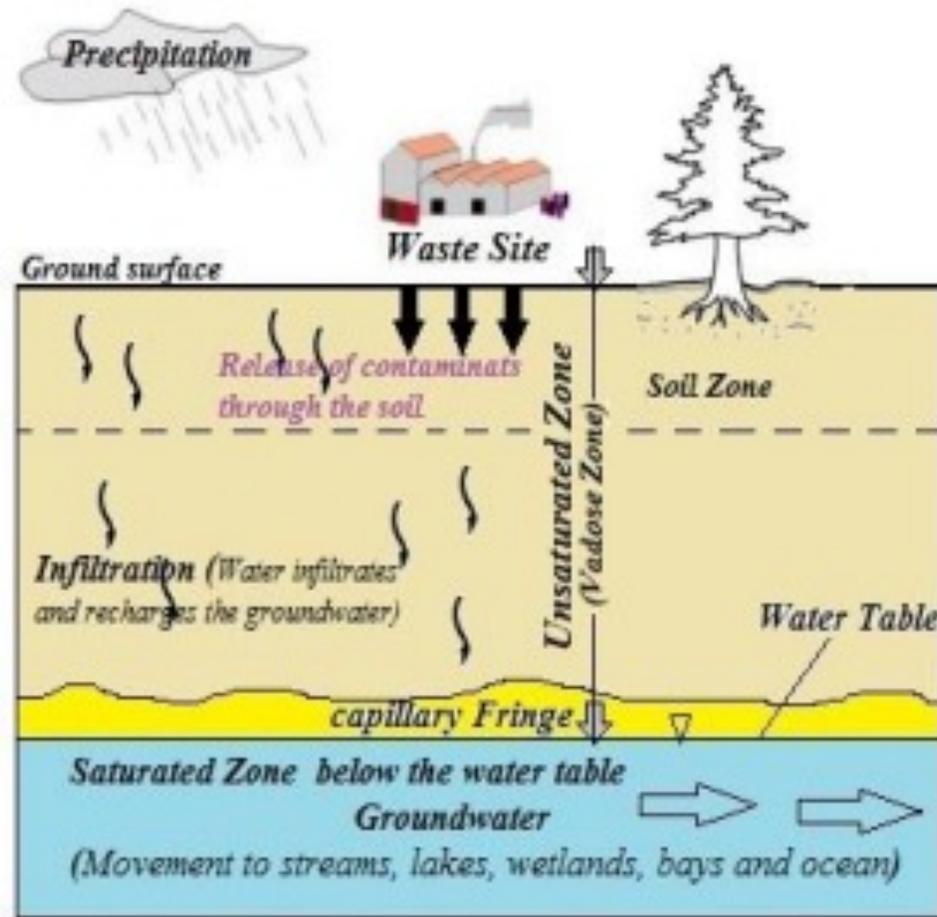


Locations of Superfund National Priorities List (NPL) in lower 48 US States (Source: U.S. EPA's *Superfund NPL Where You Live Map*, 2022)



## Basics of Soil to Groundwater (SGW) Contamination

- Occurs when a contaminant migrates through the vadose zone into the saturated zone
- Various factors affect the contaminant transport
  - Physical properties of a contaminant (e.g., vapor pressure)
  - Hydrogeologic characteristics of the soil (e.g., porosity, moisture levels, organic content, etc.)



Generic example of how contaminants move through soil into groundwater (Source: Panda & Chidambaram, 2019)

# SSL-MGW Equations for Inorganic and Organic Compounds

Equation 1- SSL-MGW for inorganic compounds  
(U.S. EPA, 1996b)

$$SSL \left( \frac{mg}{kg} \right) = C_w \cdot \left\{ K_d + \frac{\theta_w + (\theta_a \cdot H')}{\rho_b} \right\}$$

Equation 2- SSL-MGW for organic compounds (U.S. EPA, 1996b)

$$SSL \left( \frac{mg}{kg} \right) = C_w \cdot \left\{ (K_{oc} \cdot f_{oc}) + \frac{\theta_w + (\theta_a \cdot H')}{\rho_b} \right\}$$

Where:

$C_w$  = target soil leachate concentration (mg/L)

$K_d$  = Soil-water partition coefficient (L/kg)

$K_{oc}$  = Soil organic carbon-water partition coefficient (L/kg)

$f_{oc}$  = Organic carbon content of soil (kg/kg)

$\theta_w$  = Water-filled soil porosity (L<sub>water</sub>/L<sub>soil</sub>)

$\theta_a$  = Air-filled soil porosity (L<sub>air</sub>/L<sub>soil</sub>)

$H'$  = Henry's law constant (dimensionless)

$\rho_b$  = Dry soil bulk density (kg/L)

# How to Determine the Target Soil Leachate Concentration ( $C_w$ )

*Equation 3- Determination of the target soil leachate concentration ( $C_w$ ) (U.S. EPA, 1996c)*

$$C_w = (MCLG, MCL, \text{ or } HBL) \cdot DAF$$

Where:

MCLG = Maximum contaminant level goal (chemical specific concentration)

MCL = Maximum contaminant level (chemical specific concentration)

HBL = Health based limit (chemical specific concentration)

DAF= Dilution attenuation factor (dimensionless)

# Basics of the Dilution Attenuation Factor (DAF)

# DAF Definition

- ▶ U.S. EPA's 1996 SSG: User's Guide definition (U.S. EPA, 1996, p. 30)

*“As soil leachate moves through soil and ground water, contaminant concentrations are attenuated by adsorption and degradation. In the aquifer, dilution by clean ground water further reduces concentrations before contaminants reach receptor points (i.e., drinking water wells). This reduction in concentration can be expressed by a dilution attenuation factor (DAF), defined as the ratio of soil leachate concentration to receptor point concentration. The lowest possible DAF is 1, corresponding to the situation where there is no dilution or attenuation of a contaminant (i.e., when the concentration in the receptor well is equal to the soil leachate concentration). On the other hand, high DAF values correspond to a large reduction in contaminant concentration from the contaminated soil to the receptor well”*

- ▶ Simplified definition
- ▶ Default nationwide DAF of 20 (will expand throughout presentation)

# DAF Equation

*Equation 4- Calculation of the Dilution Attenuation Factor (U.S. EPA, 1996b)*

$$DAF = 1 + \left( \frac{Kid}{IL} \right)$$

*Equation 5- Calculation of aquifer mixing zone depth (U.S. EPA, 1996b)*

$$d = \sqrt{(0.0112L^2)} + d_a \left( 1 - e^{\frac{(-LI)}{(Kid_a)}} \right)$$

Where:

K= aquifer hydraulic conductivity (m/yr)

i= hydraulic gradient (m/m)

d=aquifer mixing zone depth (m)

l= infiltration rate (m/yr)

L= length of area of concern parallel to ground water flow (m)

d<sub>a</sub>= aquifer thickness (m)

$$SSL \left( \frac{mg}{kg} \right) = C_w \left\{ K_d + \frac{\theta_w + (\theta_a \cdot H')}{\rho_b} \right\}$$

$$C_w = (MCLG, MCL, \text{ or } HBL) \cdot DAF$$

$$DAF = 1 + \left( \frac{Kid}{IL} \right)$$

# History & Development of the Nationwide Default DAF

- ▶ 1<sup>st</sup> model: SSG applied the U.S. EPA Composite Model for Leachate Migration with Transformation Products (EPA CMTPL) to produce the default DAF (U.S. EPA, 1996c)
- ▶ 2<sup>nd</sup> model: Used data from two large, independent hydrogeologic surveys
  - ▶ American Petroleum Institute (API) conducted one survey and compiled data in the hydrogeologic database (HGDB)
  - ▶ U.S. EPA's data from nationwide dense non-aqueous phase liquid (DNAPL) contaminated Superfund sites

# Hydrogeologic Database (HGDB) Overview

- Raw data from the HGDB was used in models to determine nationwide DAF
- Appendix F of the U.S. EPA's 1996 SSG
- Questionnaire sent out to 8700 members of the Association of Ground Water Scientists and Engineers
- 400 “usable” responses were returned
  - Quantitative: aquifer hydraulic conductivity (K), aquifer mixing zone depth (d), infiltration rate (I), hydraulic gradient (i), etc.
  - Qualitative: location, measurement techniques, respondent position/experience, etc.



Approximate locations of HGDB survey sites; 48 out of 50 states represented (Source: Newell, Hopkins, & Bedient, 1990)

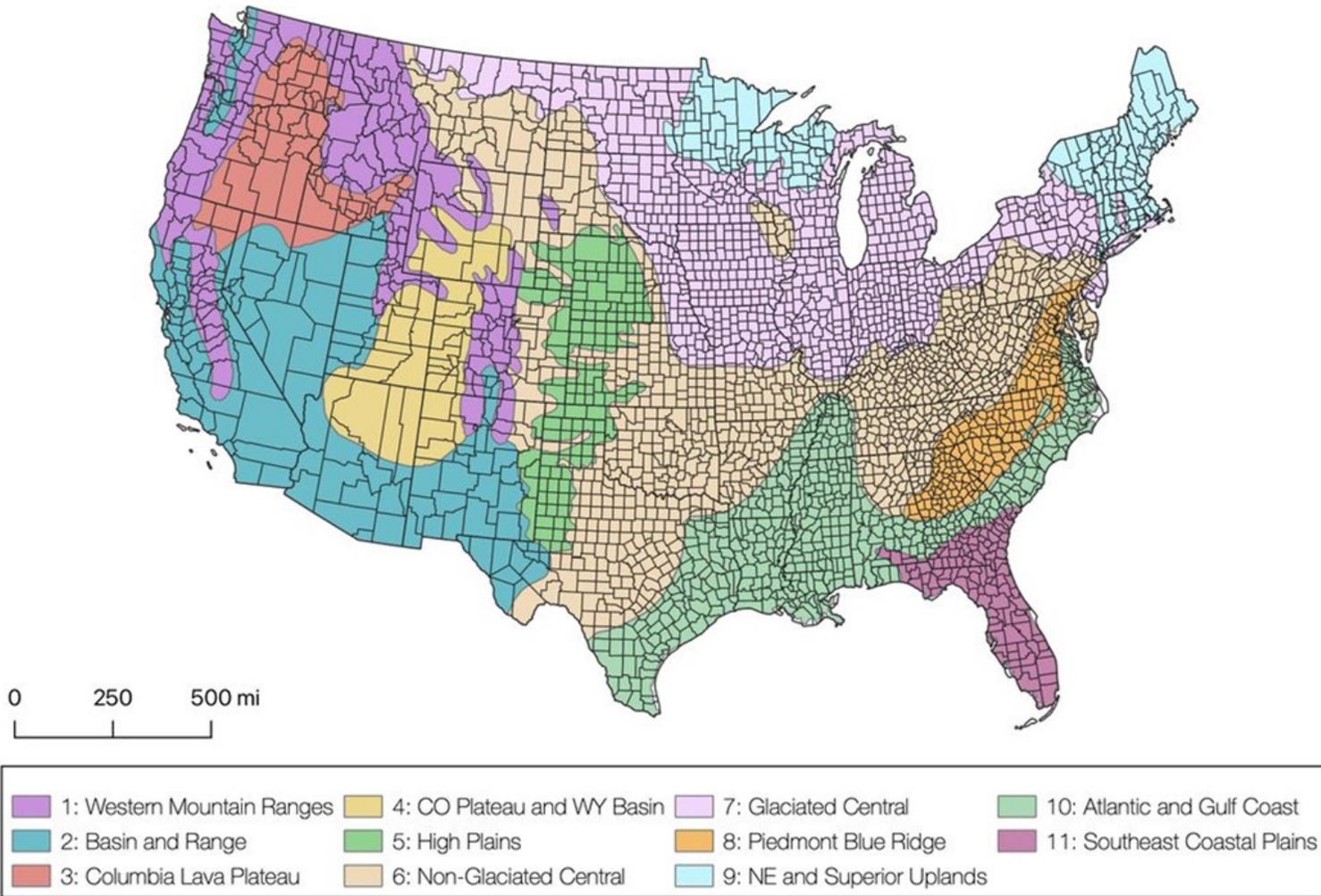
# Potential Drawbacks and Current Use of a Nationwide Default DAF

- ▶ The default DAF does not account for the large hydrogeologic variations across the country
- ▶ State Uses of DAF
  - ▶ Most states clearly stipulate using a DAF of 1 or 20
  - ▶ New Jersey calculated a state specific DAF
    - ▶ Coincidentally, the NJ specific DAF came out to 20
- ▶ DAF is currently used during the risk assessment process when calculating generic SSLs (generally, early stages of a site investigation)

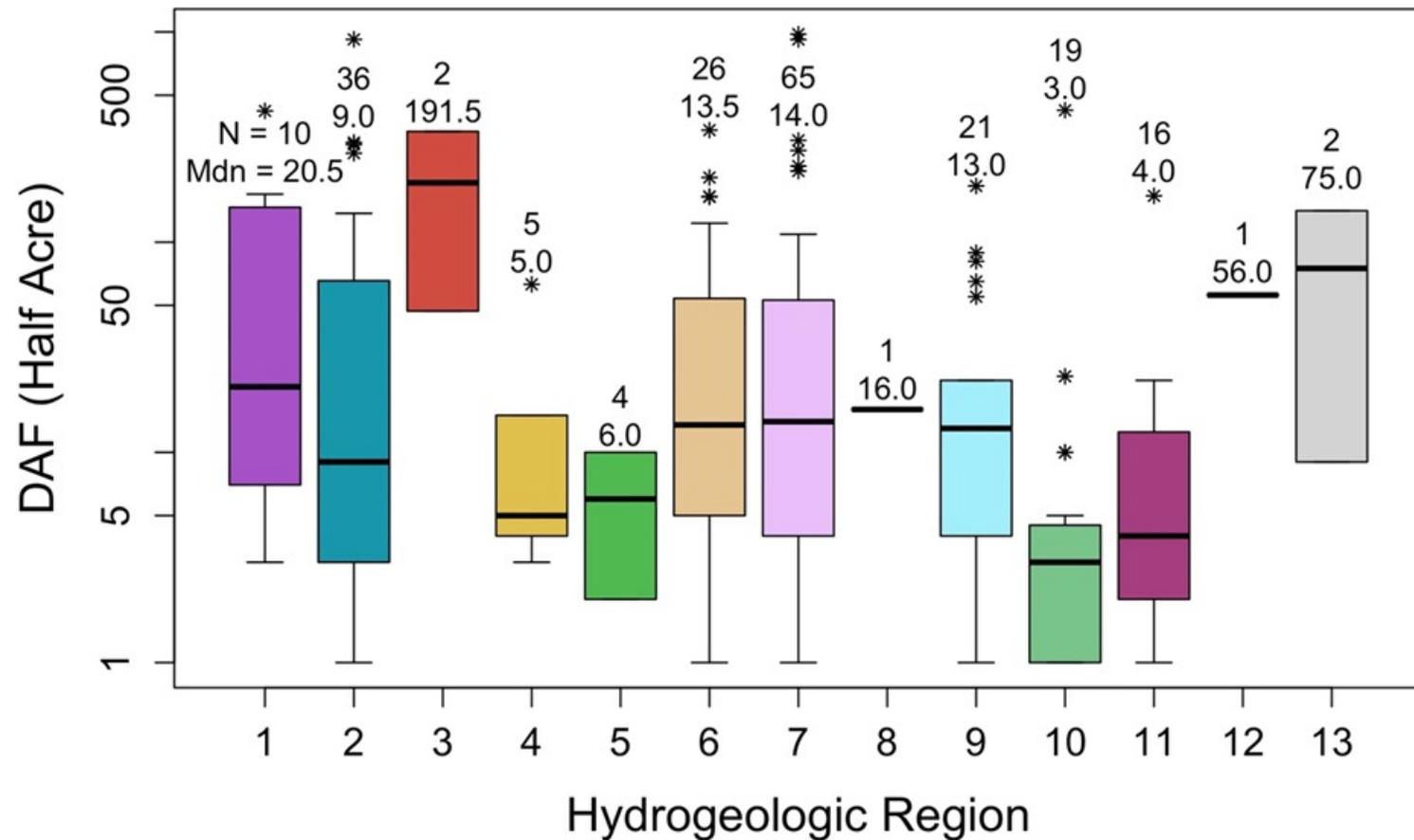
# Potential Updates to the DAF

# Hydrogeologic Region Specific DAF

- ▶ Heath (1984) identified 15 hydrogeologic regions in the United States
  - ▶ Numerous sub-regions
- ▶ HGDB contains data from 13 of these regions
  - ▶ U.S. territories were excluded due to lack of data; Alluvial Valleys defined as a sub-region in the HGDB
- ▶ Using a hydrogeologic region specific (but still generic) DAF better predicts SGW contaminant movement/dilution than a nationwide DAF



Hydrogeologic regions of the contiguous United States (12: Hawai'i and 13: Alaska not pictured). [Data from Clawges and Price \(1999\)](#)

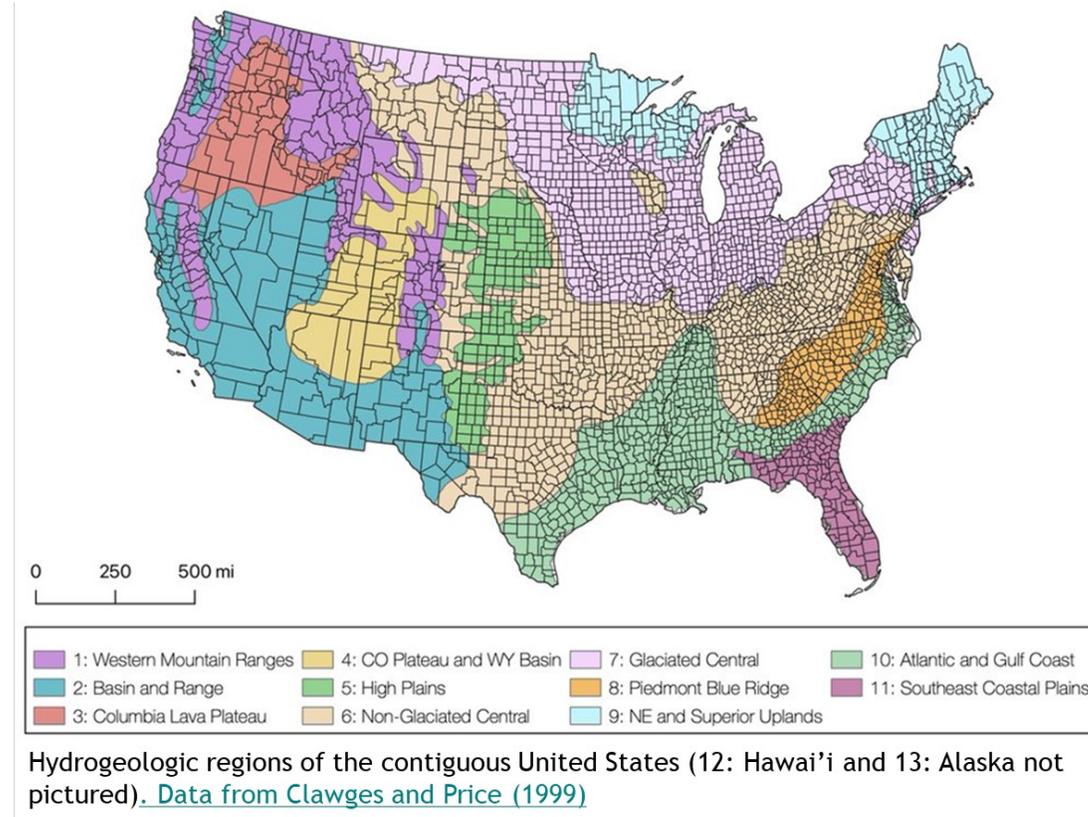


Region-specific DAFs, calculated from using HGDB data (regions correspond to Figure 2). Regions 12 and 13 refer to Hawaii and Alaska, respectively

# Regional DAF Limitations

# Identified Limitations

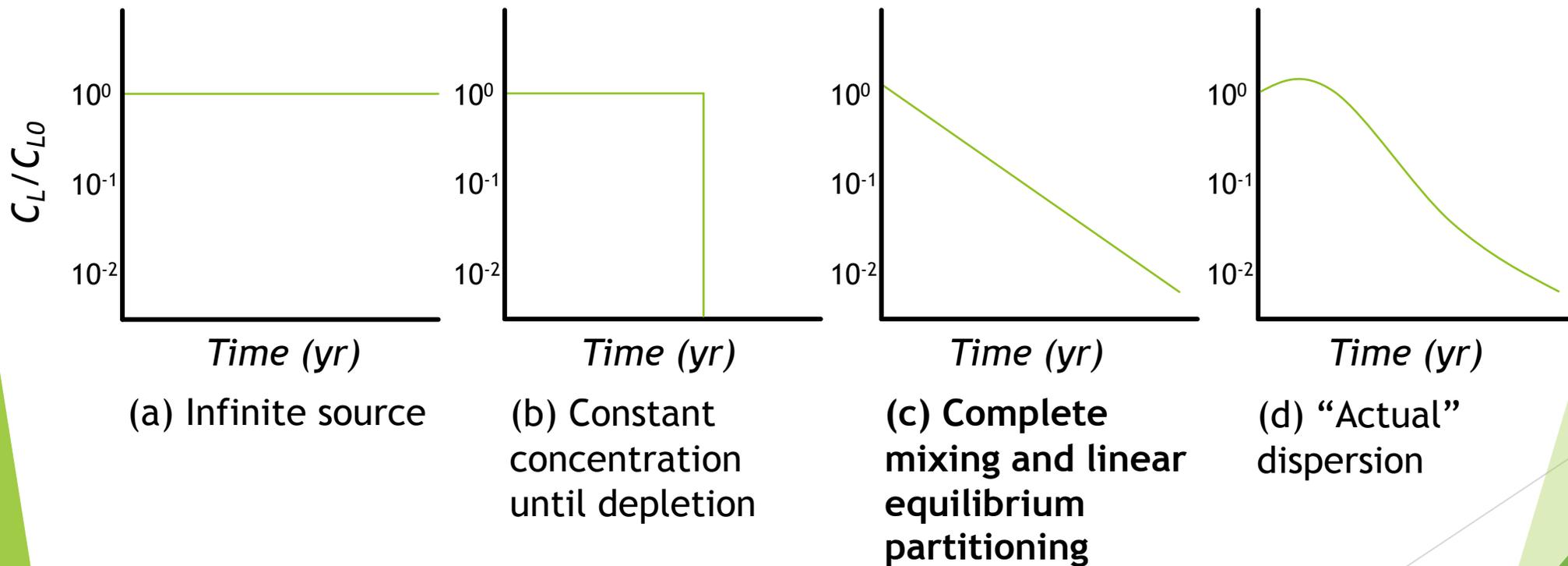
- ▶ Need more data points
- ▶ Data accuracy
  - ▶ Lack of standardized methods in original HGDB
  - ▶ Variance in estimated accuracies
- ▶ Need for GIS when determining hydrogeologic region
- ▶ Contaminant saturated soil



# Infinite Source Assumption

# Assumption and Models

- ▶ SSG assumes that “steady-state concentrations are maintained over the exposure period”



# Equation

- ▶ Dimensionless finite-source equation from Rixey et al. (2000):

$$C_{F(t^*)}/C_{\infty} = \frac{1}{2} \sqrt{\frac{Pe}{\pi}} \int_0^{t^*} \frac{-Pe[1 - (t^* - u^*)]^2 - \lambda^* u^*}{4(t^* - u^*) (t^* - u^*)^{3/2}} du^*$$

Péclet number

Source decay constant

Time

Dummy variable for integration

# Source Decay Constant

- ▶ The source decay constant ( $\lambda^*$ ) captures chemical- and site-specific data:

$$\lambda^* = \frac{ILR}{dF_w\rho_wK_dv_x}, \text{ where}$$

- I = infiltration rate (m/yr)
  - EPA default: 0.28 m yr<sup>-1</sup>
- L = length to receptor well (m)
  - EPA default: 45 m
- R = retardation factor (unitless)
  - Chemical specific
- d = depth of aquifer (m)
  - EPA default: 15 m
- F<sub>w</sub> = fraction of waste in the landfill (float between 0 and 1)
  - No EPA default
- $\rho_w$  = chemical density (kg/L)
  - Chemical specific
- K<sub>d</sub> = solid-aqueous partition coefficient (L/kg)
  - Chemical and site specific
- v<sub>x</sub> = groundwater velocity (m/yr)
  - EPA default: 158 m yr<sup>-1</sup>

# Calculator

- ▶ Calculator available at [growingecology.com/finite-source](http://growingecology.com/finite-source)

## Finite Source Correction Factor Calculator

The Finite Source Correction Factor calculator was developed for an internship with U.S. EPA Office of Land and Emergency Management studying potential updates to the soil-to-groundwater pathway Soil Screening Level (SSL). To convert between an infinite-source SSL and a finite-source SSL, simply multiply the infinite-source DAF by the correction factor.

<h3>Chemical Specific</h3> <p>Chemical Name</p> <input type="text" value="Select one"/>	<h3>Site Specific</h3> <p>Organic Carbon Fraction</p> <input type="text" value="0.002"/>	<h3>Result</h3> <p>The finite-source correction factor for <b>none selected</b> is <b>1.0</b>.</p> <input type="button" value="Calculate"/>
<p>Values for PFAS and PFOAS are provisional and included solely for demonstration.</p> <p><b>Optional:</b></p> <p>The dropdown menu automatically updates the following values, so you only need to enter them manually if they differ from those stored in the database.</p> <p><math>K_{oc}</math></p> <input type="text" value="40.0"/> <p>Liters per kilogram</p> <p>Chemical Density</p> <input type="text" value="1.0"/> <p>Kilograms per liter</p>	<p>Number between 0 and 1</p> <p>Infiltration Rate</p> <input type="text" value="0.28"/> <p>Meters per year</p> <p>Length to Receptor Well</p> <input type="text" value="45"/> <p>Meters</p> <p>Depth to Aquifer</p> <input type="text" value="15"/> <p>Meters</p> <p>Fraction of Waste in the Landfill</p> <input type="text" value="0.05"/>	

# Relation to DAF

- ▶ Simply multiply DAF by correction factor
- ▶ For example, at a site where 5% of the soil is contaminated with vinyl chloride and all other values are the EPA default,

Finite Source Correction Factor = 3.96

Steady-state DAF = 20 (default)

Finite DAF = 79.2

$$C_{W-FS} = (MCLG, MCL, \text{ or } HBL) \cdot DAF \cdot CF_{FS}$$

# Finite-Source Correction Limitations

# Identified Limitations

- ▶ Rixey et al. may be outdated
- ▶ Need to integrate regionalized default values
- ▶ Dependent on accurate inputs (e.g.,  $K_d$ )
- ▶ Would affect ability to compare SSL with other MCLs

# Future Work

# Expanding the hydrogeologic database with NPL sites and other relevant data

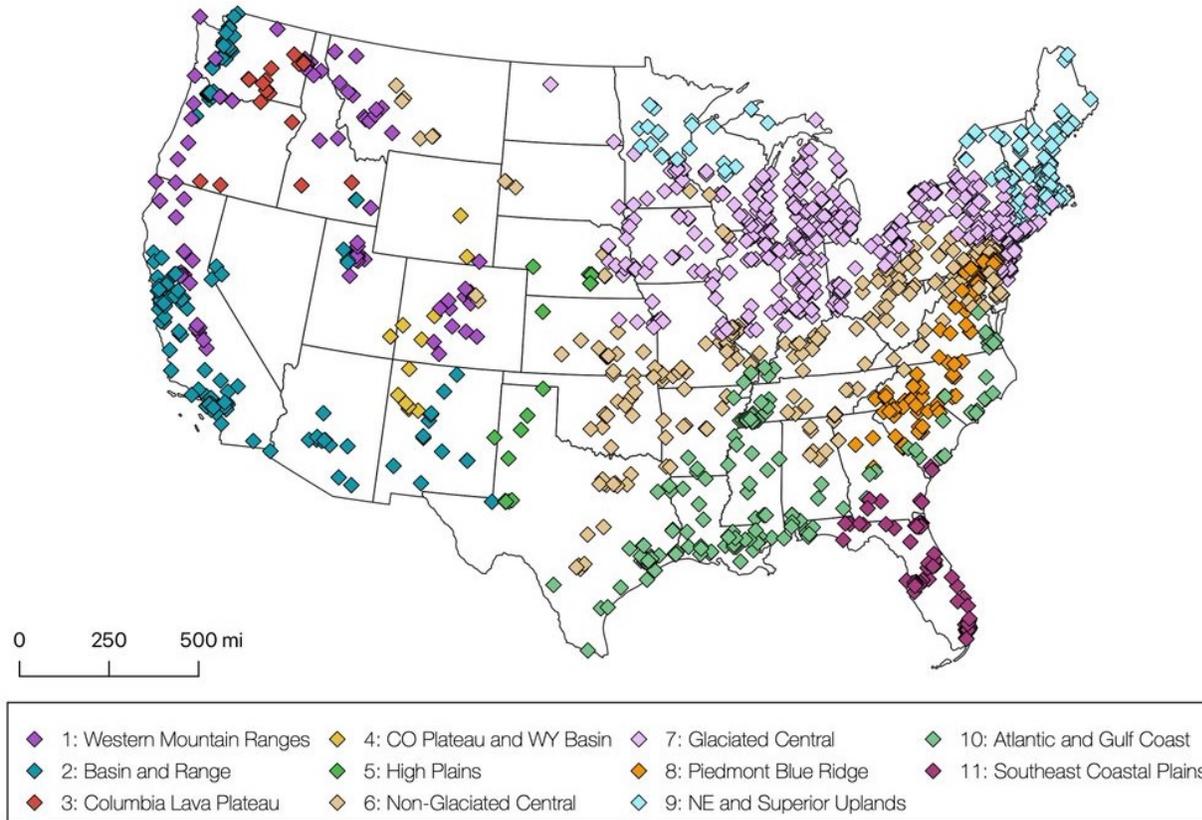


Figure 4: NPL sites by hydrogeologic region (12: Hawaii and 13: Alaska not pictured). Hydrogeologic region data from Clawges and Price (1999); Superfund site locations from US EPA (2022)

# Replicating/Checking Original HGDB Survey

- ▶ Replicating the original surveys with standardized techniques/data collection methods and quality control
  - ▶ Likely expensive and require significant resources/coordination
- ▶ Alternatively, using “spot checks” of certain sites could determine the magnitude of data variance/error in the HGDB

# Eliminating other assumptions and gaps

- ▶ No NAPLs present (if NAPLs are present, the SSLs do not apply)
- ▶ No contaminant attenuation (i.e., adsorption, biodegradation, chemical degradation) in soil or aquifer
- ▶ PFAS

# Conclusion



**CONTACT INFO:**

Michael McCarroll @ [mccarroll.Michael@epa.gov](mailto:mccarroll.Michael@epa.gov)

Alex Valdez @ [alivaldez92@gmail.com](mailto:alivaldez92@gmail.com) for general questions

Seth Whiteaker @ [sjwhiteaker@ucdavis.edu](mailto:sjwhiteaker@ucdavis.edu) for general questions, data, and code