

ChemFate Model 1.0

User Guide

Keller Lab – Assessment of Risk and Information System (KLARIS)

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1. Introduction

The ChemFate model is a dynamic (level IV) multimedia mass balance model, which is designed to predict time-dependent (daily) concentrations in the environment for four kinds of chemicals: (1) non-ionizable organic chemicals (OrganoFate); (2) ionizable organic chemicals (ionOFate); (3) metals (metalFate); (4) nanomaterials (NanoFate). The model can be used as a standalone analysis as well as in risk and life cycle assessment of chemicals. This dynamic tool can be applied to study emerging and existing organic contaminants such as pesticides, pharmaceuticals, chemicals in personal care products, and metals in paints. Fugacity is used as an equilibrium criterion for non-ionizable organic chemicals, equivalence is used for ionizable organic and metals, and concentration is used for nanomaterials.

The model tracks the neutral form for non-ionizable organic chemicals. For ionizable organic chemicals, it keeps track of the neutral and primary ionic forms over time in the environment. The fact that the ionic form of certain chemicals should be more toxic than the neutral form emphasizes the need for comprehensively assessing the environmental risks of ionizable chemicals. Therefore, for ionizable organic chemicals, the users can run the model as either ionizable or not and compare the concentration differences. For metals, the model tracks concentrations in three phases: particulate, colloidal, and dissolved. Metal in the colloidal phase is defined as the metal bound to dissolved organic matter. For nanomaterials, the model tracks three engineered nanomaterial (ENM) states: free nanoparticles and small homoaggregates, ENM particles heteroaggregated with aerosols or suspended sediments, ENM dissolution products in the various waters.

The unique thing about ChemFate is that it allows one to model region variations, since the distribution of a chemical is highly dependent on the relative volumes of different environmental media compartments (e.g. atmosphere, freshwater, coastal water, soil types), climate (e.g. precipitation, temperature, wind speed), and other local factors (e.g. chemical use and release, wastewater treatment, solid waste handling). The model was developed in Python and is hosted in Github at <https://github.com/klaris-ak/ChemFate>.

1.1 Model Input Files

ChemFate is fully customizable – for any region, its climate variability and time-dependent releases can be modeled over any length of time. Complexity of the environment is captured in nine key (bulk) compartments (air, freshwater and freshwater sediment, marine water and marine sediment, and four soil types). These can be further sub-divided as needed, for a total of twenty-six distinct environmental compartments for a given geographic region. The characteristics of each compartment are specified with a number of parameters that define the dimensions and characteristics of each.

Broadly, six categories of data are required to run ChemFate. These are stored in three excel files located in the “ChemFate/Input” folder:

1. Chemical property information - Data on intrinsic chemical behavior in the environment (“ChemProp.xlsx”)
 - a. “ChemParam_non-ionizableOrganic.xlsx” contains the chemical parameters that are needed for non-ionizable organic chemicals.
 - b. “ChemParam_ionizableOrganic.xlsx” contains the chemical parameters that are needed for ionizable organic chemicals
 - c. “ChemParam_metal.xlsx” contains the parameters that are specific for metals.
 - d. “ChemParam_nanomaterial.xlsx” contains the parameters that are specific for nanomaterials.
2. Climate information - Data on climate specific to the region of interest, including daily temperature (°C), precipitation (mm/day), freshwater flow (m³/second), wind speed (m/second), and evaporation (mm) (“Region.xlsx”, sheet “Climate”)
3. Geographic characteristics - Data on land use types, soil properties, environmental media properties, etc. (“Region.xlsx”, sheet “Environment”)
4. Presence or absence of a bulk environmental compartment at the location of interest (“Region.xlsx”, tab “Presence”)
 - a. In some regions, certain compartments are unnecessary (e.g. no marine compartment in a land-locked region). The user can specify the presence (1) or absence (0) of specific compartments. The transport processes and calculations are adjusted accordingly. The user can also adapt these compartments, for example by considering a receiving freshwater water body instead of a marine compartment.
5. Chemical Release - Data on (temporal) trends of product/chemical release amount to the region of interest (“ChemRelease.xlsx”, sheet “Release”)
6. Background concentration - Data on existing/current presence of chemical in different environmental media at the region of interest (“ChemRelease.xlsx”, sheet “bgConc”)

1.2 Model Outputs

ChemFate models the transport and transformation of chemicals in the environment and predicts the daily mass, concentration, and form of the chemical in each compartment. ChemFate creates the following outputs:

Daily concentration of each chemical’s various forms (if applicable) in each compartment	XLSX file
Daily mass of each chemical’s various forms (if applicable) in each compartment	XLSX file
Daily total mass transfer for each transport process	XLSX file
Heatmap showing comparison of each chemical’s overall average concentration for all compartments	Jpeg

Line graphs showing each chemical's concentration variability over time	Jpeg
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2. Model Configuration

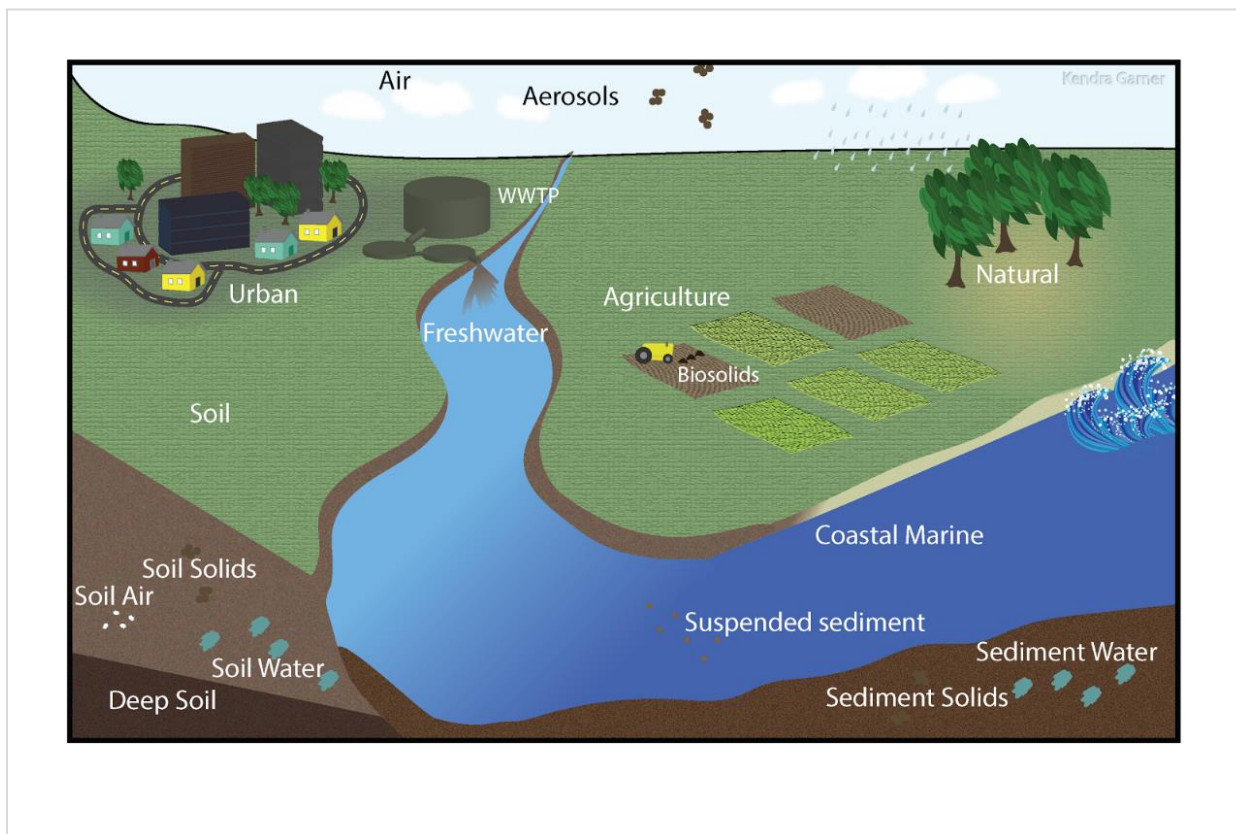
2.1 The Environment

The environment is composed of nine bulk compartments (e.g., atmosphere, freshwater, and agricultural soil), which in turn have a number of subcompartments (e.g. soil air, soil water and soil solids) (Table 1). Figure 1 shows the conceptual model of all compartments in a region. Each subcompartment has dimensions, densities and characteristics that describe its specific medium. Each medium is assumed to be a homogenous box and characterized using parameters that are unique to its geographical region. The “Biosolids Agriculture Soil” is intended to account for the application of wastewater sludge (biosolids) to agricultural soil, if the practice is locally permitted.

Table 1. Compartments (in blue) and subcompartments included in ChemFate.

Atmosphere	Freshwater	Urban soil
Air	Fresh water column	Air in urban soil
Aerosols	Freshwater suspended sediment	Water in urban soil
	Freshwater sediment bed	Urban soil solids
	Water in freshwater sediment	Deep urban soil
	Solids of freshwater sediment	Undeveloped soil
	Coastal marine	Air in undeveloped soil
	Marine water column	Water in undeveloped soil
	Marine water suspended sediment	Urban undeveloped solids
	Marine sediment bed	Deep undeveloped soil
	Water in marine sediment	Agricultural soil
	Solids of marine sediment	Air in agricultural soil
		Water in agricultural soil
		Urban agricultural solids
		Deep agricultural soil
		Biosolids agricultural soil
		Air in biosolids agricultural soil
		Water in biosolids agricultural soil
		Urban biosolids agricultural solids
		Deep biosolids agricultural soil

Figure 1. ChemFate compartments and subcompartments (drawn by Dr. Kendra Garner)



2.2 Available Default Environment

A selection of default environments are available in ChemFate that represent a range of distinct climate conditions and land use types. This was developed so the users can quickly evaluate the environmental fate of a chemical without the investment in data collection of regional characteristics. These regions are meant to provide distinct characteristic environments that can be substituted for similar regions. There are twelve default environments, including eight regions in the United States and four regions in the Europe, and one global environment (Table 2). For instance, Des Moines in Iowa is representative of a region with heavy agriculture area, while New York City represents a region with a high proportion of urban area. A global environment was developed for the users who are interested in a broader scope; average parameter values at this scale have not been verified. Maps of those default regions are presented in Appendix I.

Table 2. The list of default environments available to use.

Region	State	Country
Austin	Texas	United States
Des Moines	Iowa	United States
Los Angeles	California	United States
San Francisco	California	United States

Visalia	California	United States
Upper Santa Clara River Watershed	California	United States
San Joaquin River Watershed	California	United States
Salem	Oregon	United States
New York City	New York	United States
London		United Kingdom
Rome		Italy
Stockholm		Sweden
Zurich		Switzerland
Global Environment		

2.3 Environmental Parameters

The following tables show the environmental parameters required to run the model. Each table contains name of the parameter, unit of measurement and if this parameter is specific to ionizable chemicals. If a parameter is only used for ionizable chemicals (ionizable organic chemicals and metals), and the chemical of interest is a non-ionizable organic chemical, the value of this parameter can be left empty. Column “G or L”, indicating if the parameter is set to a general value (G) or varies by location (L) and is a required user input. The general (default) values are derived from the literature. The values that are region-specific are indicated with an “L” and the tables show parameter values specific to the San Francisco Bay area (Table 3 to Table 7).

Soils can be divided into four major land use categories or four different landcover types (e.g. row crop, pasture, urban, and undeveloped) depending on the needs of the user. Within each land use type, the soil properties are spatially-averaged based on the predominant soil type. These values will vary significantly from region to region. Section 6 outlines the process for obtaining parameter values for your region of interest should you opt not to use a default environment. Furthermore, the users can alter the default environments if they are interested in a smaller region or different climate.

2.3.1 Atmosphere

The atmosphere contains two subcompartments, a gaseous air phase and an aerosol subcompartment. The atmosphere height is adjustable, depending on typical local meteorological conditions, though generally assumed to be the first 1,000 m above the land surface. It can be adjusted in case there are frequent thermal inversions. Other parameters required to describe air characteristics are listed Table 3.

2.3.2 Aerosols

Aerosols can be mostly water vapor (e.g., fog), mineral (e.g., dust) or organic (e.g., broken leaf materials, microbes). By default, the model assumes aerosols to be composed of water vapor (50%) and suspended solids (50%). The user can modify the properties of the aerosol compartment to best describe local conditions. The local concentration of aerosols is based on PM10 (particulate matter less than 10 micrometers) measurements.

Table 3. Parameters used to characterize 'air and aerosol compartments'

Parameter	G or L	Value	Units
Air Height	G	1.00×10^3	m
Air Density	G	1.19	kg/m ³
Dynamic Viscosity of Air	G	1.85×10^{-5}	kg/m-s
Aerosols Density	G	1.80×10^3	kg/m ³
Aerosols Concentration	L	3.00×10^{-8}	kg/m ³
Aerosol Water pH	G	5.55	-
Aerosol Organic Carbon Content	G	0.10	kg/kg
Average Aerosols Particle Radius	G	2.50×10^{-6}	m
Wet Deposition Aerosols Scavenging Ratio	G	2.00×10^{-5}	-

2.3.3 Water Compartments

ChemFate separates surface water into two bulk compartments – freshwater and coastal marine water. The freshwater compartment includes all surface overland water such as rivers, streams and lakes. The coastal marine compartment receives the outflowing water from the freshwater compartment, and the flow is then routed out of the model, with a net loss of chemical to deeper ocean waters. Table 4 outlines the parameters required for describing freshwater and marine compartments respectively. As with air, the user can customize these parameters. The user can also modify the parameters describing freshwater and marine compartments to account for any two connected water bodies (e.g. near field and far field, or a system with a river and a lake). The marine compartment can also be treated as an estuarine area but need to be downstream of the freshwater compartment.

Some landlocked regions such as Des Moines, Iowa or Salem, Oregon contain only a freshwater compartment. In this case, the user has the ability to exclude the marine compartment in the input file 'Region.xlsx', tab 'Presence'. Release of a chemical to the environment after passing through the local wastewater treatment plants (WWTP) is dependent on the location of the WWTPs, i.e. whether it discharges to freshwater or the marine environment. The user should assign the proportion of WWTP release to each water compartment (freshwater or marine) based on WWTP flowrates.

Table 4. Parameters used to characterize water bodies

Parameter of each water type	G or L	Freshwater	Marine water	Units
		Value	Value	
Area	L	1.59×10^9	1.65×10^8	m ²
Depth	L	1.00	6.00	m
Density	G	1.00×10^3	1.03×10^3	kg/m ³
Dynamic Viscosity	G	1.00×10^{-3}	1.00×10^{-3}	kg/m-s

2.3.4 Suspended Sediments

Suspended sediments are modeled in each water compartment. The parameters used to define their properties are shown in Table 5. The organic carbon content is particularly important, since it determines adsorption capacity for most organic chemicals.

Table 5. Parameters used to characterize suspended sediments

Parameter in each water type	G or L	Freshwater	Marine water	Units
		Value	Value	
Suspended Sediment Density	G	1.50×10^3	1.50×10^3	kg/m ³
Suspended Sediment Concentration	L	1.00×10^{-2}	5.00×10^{-3}	kg/m ³
Average Suspended Sediment Particle Radius	G	1.00×10^{-6}	1.00×10^{-6}	m
Suspended Sediment Organic Carbon Content	L	1.50×10^{-1}	2.30×10^{-1}	-

2.3.5 Sediments

Sediments refers to the sediment bed in each water compartment. The parameters used to define their properties are presented in Table 6. Most top-layer sediments contain a significant fraction of water (e.g. 80%), and that is reflected in the solid fraction. A certain fraction of the sediment is buried deeper, with less accessibility, which is modeled with a constant burial rate. There is also a constant resuspension rate for the top-layer sediment bed, which returns sediments to the water column as suspended sediment. The sediment bed moves along with the flow of water, with an assumed flow ratio (e.g. freshwater sediment is assumed to flow at 0.005% of the freshwater flow).

Table 6. Parameters used to characterize sediments

Parameter in each water type	G or L	Freshwater	Marine water	Units
		Value	Value	
Sediment Depth	L	5.00×10^{-2}	2.50×10^{-1}	m
Density of Sediment Solid	G	2.40×10^3	2.40×10^3	kg/m ³
Sediment Solid Ratio	L	2.00×10^{-1}	2.00×10^{-1}	-
Sediment Organic Carbon Content	L	5.00×10^{-2}	8.00×10^{-2}	-
Burial Rate for Sediment	G	4.19×10^{-8}	4.50×10^{-8}	m ³ /m ² -hr
Resuspension Rate for Sediment	G	3.00×10^{-7}	2.00×10^{-7}	m ³ /m ² -hr
Sediment Advective Flow Ratio	G	5.00×10^{-5}	5.00×10^{-5}	-

2.3.6 Soils

Soils can be divided into four major land use categories or four different landcover types (e.g. row crop, pasture, urban, and undeveloped) depending on the needs of the user. Within each land use type, the soil properties are spatially-averaged based on the predominant soil type.

2.3.6.1 Urban Area

The urban regions include developed high intensity (e.g., apartment complexes, row houses, commercial or industrial regions), developed medium intensity (e.g., single family house units), developed low intensity (e.g., single family houses with large plots of land). These areas have low permeability since a large fraction is paved or covered.

2.3.6.2 Undeveloped Area

Undeveloped regions include barren land, deciduous forests, evergreen forests, mixed forests, scrub, shrub, grassland/herbaceous, and wetlands.

2.3.6.3 Agricultural Area

The agricultural regions include both pasture and cropland.

2.3.6.4 Agricultural Area Subject to Biosolids Application (Biosolids Soil)

Many countries allow the application of biosolids (residuals generated from wastewater treatment plant processes) to agricultural fields. After WWTPs, those chemicals may still be present in the biosolids. Through biosolids, these chemicals can then accumulate in soils, and may result in indirect exposure to humans and other organisms via food. Thus, in ChemFate, we provide the user the ability to model those agricultural areas subject to biosolids application. The user can also model a different type of agriculture or soils, with or without biosolids.

Table 7. Parameters used to define soils – air in soil, water in soil, soil solids and deep soil

Parameter in each soil type	G or L	Soil 1 (Undeveloped)	Soil 2 (Urban)	Soil 3 (Agricultural)	Soil4 (Biosolids Applied)	Units
Soil Area	L	7.58×10^9	3.49×10^9	1.51×10^9	7.97×10^7	m ²
Cation Exchange Capacity on Surface Soil	L	13.8	12.2	12.4	12.4	-
Depth Surface Soil	L	0.358	0.38	0.393	0.393	m
Density of Soil Solid	G	2400	2400	2400	2400	kg/m ³
Initial Soil Water Content	L	0.3	0.3	0.4	0.4	-
Soil Water pH	L	7.16	7.79	8.04	8.04	-
Initial Soil Air Content	L	0.20	0.20	0.20	0.20	-
Organic Carbon Content Soil	L	5.90×10^{-2}	3.10×10^{-2}	5.90×10^{-2}	5.90×10^{-2}	-
Runoff Curve Number for Soil	G	82.2	91.0	91.0	91.0	-

Field Capacity	L	0.32	0.14	0.32	0.32	m ³ / m ³
Depth Deep Soil	G	1.0	1.0	1.0	1.0	m
Cation Exchange Capacity on Deep Soil	L	13.8	12.2	12.4	12.4	-
Density of Deep Soil Solid	G	2.50×10 ³	2.50×10 ³	2.50×10 ³	2.50×10 ³	kg/m ³
Deep Soil Organic Carbon Content	L	1.00×10 ⁻³	1.00×10 ⁻³	1.00×10 ⁻³	1.00×10 ⁻³	-
Saltation Fitting Parameter	G	1.00	1.00	1.00	1.00	-
Threshold Wind Velocity to Cause Erosion	L	0.716	1.42	0.55	0.55	m/s
Minimum Threshold Shear Velocity	L	30.0	30.0	30.0	30.0	m/s
Height of Wind Measurements	G	1.50	1.50	1.50	1.50	m
Roughness of Soil	G	2.40×10 ⁻³	6.00×10 ⁻¹	1.00×10 ⁻¹	1.00×10 ⁻¹	m
Kconstant for Soil	L	2.00×10 ⁻²	2.00×10 ⁻⁴	3.16×10 ⁻³	3.16×10 ⁻³	m ⁻¹
Hours per Day of Sufficient Wind for Wind Erosion	G	4.17×10 ⁻¹	4.17×10 ⁻¹	4.17×10 ⁻¹	4.17×10 ⁻¹	h/24h
Consistency of Wind Throughout the Day	G	0.05	0.05	0.05	0.05	-
Percent Land Uncovered and Available for Wind Erosion	G	0.05	0.05	0.05	0.05	-

Percent Particles that Remain Suspended Based on Average Soil Size Distribution	G	0.10	0.10	0.10	0.10	-
Soil Erodibility Factor (K)	L	0.286	0.29	0.306	0.306	-
Slope	L	11.7	11.9	8.38	8.39	-
Crop Management Factor	L	2.62×10^{-2}	1.50×10^{-1}	3.00×10^{-1}	3.00×10^{-1}	-
Support Practice Factor	L	0.50	0.30	0.60	0.60	-
Leaching Rate	G	6.25×10^{-5}	6.25×10^{-5}	6.25×10^{-5}	6.25×10^{-5}	$\text{m}^3/\text{m}^2\text{-hr}$

3. Fate and Transport Processes

This user guide is focused on non-ionizable organic chemicals, ionizable organic chemicals and metals. Please refer to a previous publication for nanomaterials (Garner et al., 2017).

To estimate the behavior of chemical substances, fugacity is used for non-ionizable organic chemicals, while equivalence is used for ionizable organic chemicals and metals. The concept of fugacity was first defined by Mackay (Mackay and Paterson, 1981) based on the behavior of ideal gases to model the fate of chemicals in the environment. However, fugacity is not suitable for predicting the fate of involatile chemicals, such as ionic species or metals (Mackay and Diamond, 1989). Equivalence was introduced as an equilibrium criteria for ionizable chemicals, along with a pseudo single species mass balance modeling technique for multi-species chemicals (Diamond et al., 1992). Both fugacity and equivalence are linearly related to concentration through the chemical capacity Z values and D values, which are used to quantify transport and transformation rates for all chemicals (Csiszar et al., 2011; Diamond et al., 1992).

3.1 Concentration and Z Values

The concentration C (mol/m^3) of a non-ionizable organic chemical species can be calculated using fugacity (Pa) and fugacity capacity Z_f ($\text{mol}/\text{m}^3\text{-Pa}$). For ionizable chemicals it can be calculated using equivalence Q (mol/m^3) and equivalence capacity Z_Q (dimensionless). Those two relationships are described by $C = fZ_f$, and $C = QZ_Q$, where Z values are calculated using phase partition coefficients (e.g., $K_{aw} = \frac{Z_{air}}{Z_{water}}$, so $Z_{water} = \frac{Z_{air}}{K_{aw}}$).

Z_Q values for ionizable chemicals are species-specific and can be calculated for each phase and compartment. By definition, Z_Q values for all water phases are equal to 1 for any species. Each bulk compartment contains multiple phases or subcompartments, such as gas, water, and solids in air and soils. Within each bulk compartment, equilibrium is assumed for each species.

3.1.1 Z Values for Non-ionizable Organic Chemicals

Z values for non-ionizable organic chemicals are calculated from Mackay, 2001, and are in units of mol/Pa-m³.

3.1.1.1 Air Phase - Z_{air}

$$Z_{air} = \frac{1}{T \times R}$$

Where T is temperature in Kelvin and R is the gas constant 8.314 in Pa-m³/mol-K.

3.1.1.2 Water Phase - Z_{water}

$$Z_{water} = \frac{Z_{air}}{K_{aw}}$$

The Z value for water phase can be calculated using Z_{air} and air-water partition coefficient K_{aw} .

3.1.1.3 Solid Phase

3.1.1.3.1 Aerosol - Z_{aero}

$$Z_{aero} = Z_{air} \times K_p \times \rho_{aero} \times 10^9$$

Where K_p is aerosol-air partition coefficient in m³/μg, ρ_{aero} is the density of aerosol in kg/m³, and 10⁹ is for the unit conversion between kg and μg.

3.1.1.3.2 Suspended Sediment - Z_{sussed}

$$Z_{sussed} = Z_{water} \times K_{oc} \times f_{oc-sussed} \times \frac{\rho_{sussed}}{1000}$$

Where K_{oc} is organic carbon-water partition coefficient in L/kg, $f_{oc-sussed}$ is organic carbon content of suspended sediment in kg/kg, and ρ_{sussed} is density of suspended sediment in kg/m³.

3.1.1.3.3 Sediment Solid - $Z_{sedsolid}$

$$Z_{sedsolid} = Z_{water} \times K_{oc} \times f_{oc-sedsolid} \times \frac{\rho_{sedsolid}}{1000}$$

Where K_{oc} is organic carbon-water partition coefficient in L/kg, $f_{oc-sedsolid}$ is organic carbon content of sediment solid in kg/kg, and $\rho_{sedsolid}$ is density of sediment solid in kg/m³.

3.1.1.3.1 Soil Solid - $Z_{soilsolid}$

$$Z_{soilsolid} = Z_{water} \times K_{oc} \times f_{oc-soil} \times \frac{\rho_{soil}}{1000}$$

Where K_{oc} is organic carbon-water partition coefficient in L/kg, $f_{oc-soil}$ is organic carbon content of soil in kg/kg, and ρ_{soil} is density of soil solid in kg/m³.

3.1.1.4 Bulk Air - $Z_{air-bulk}$

$$Z_{air-bulk} = Z_{air} \times (1 - V_{f,aero}) + Z_{aero} \times V_{f,aero}$$

Where $V_{f,aero}$ is volume fraction of aerosol.

3.1.1.5 Bulk Water - $Z_{water-bulk}$

$$Z_{water-bulk} = Z_{water} \times (1 - V_{f,sussed}) + Z_{sussed} \times V_{f,sussed}$$

Where $V_{f,sussed}$ is volume fraction of suspended sediment.

3.1.1.6 Bulk Sediment - $Z_{sed-bulk}$

$$Z_{sed-bulk} = Z_{water} \times (1 - V_{f,sedsolid}) + Z_{sedsolid} \times V_{f,sedsolid}$$

Where $V_{f,sedsolid}$ is volume fraction of sediment solids.

3.1.1.7 Bulk Soil - $Z_{soil-bulk}$

$$Z_{soil-bulk} = Z_{air} \times V_{f,soil\ air} + Z_{water} \times V_{f,soil\ water} + Z_{sedsolid} \times (1 - V_{f,soil\ air} - V_{f,soil\ water})$$

Where $V_{f,soil\ air}$ is volume fraction of soil air and $V_{f,soil\ water}$ is volume fraction of soil water.

3.1.2 Z Values for Ionizable Organic Chemicals

Z values for ionizable chemicals are species-specific and are usually generated from species-specific partition coefficients. Z values for ionizable chemicals are unitless.

3.1.2.1 Air Phase - Z_{air}

$$Z_{air,n} = K_{aw,n} \times Z_{water,n}$$

Where $K_{aw,n}$ is air-water partition coefficient of the neutral form of a chemical and $Z_{water,n}$ is defined as 1.

$$Z_{air,i} = 0$$

Since ionized chemicals are assumed not to transfer from water to air, the air-water partition coefficient of ions ($K_{aw,i}$) is 0. Therefore, $Z_{air,i}$ is 0.

3.1.2.2 Water Phase - Z_{water}

$$Z_{water,n} = Z_{water,i} = 1$$

All Z values for water phase species are equal to 1 by definition.

3.1.2.3 Solid Phase

$$\begin{aligned} Z_{solid,n} &= K_{d,n} \times Z_{water,n} = K_{d,n} \\ Z_{solid,i} &= K_{d,i} \times Z_{water,i} = K_{d,i} \end{aligned}$$

Where $Z_{water,n}$ and $Z_{water,i}$ are equal to 1. Calculations of $K_{d,n}$ and $K_{d,i}$ are detailed in Section 3.3.2.

3.2 Speciation for Ionizable Chemicals

ChemFate is designed to track two states of ionizable organic chemicals: 1) the neutral form of the chemical; and 2) the primary ionic form of the chemical. We assume that an equilibrium exists between the neutral and ionic species, so the species concentration fractions (denoted as X values) are constant in each compartment for a given day. As a result, the equations for multispecies can be simplified to pseudo-single-species mass balance equations (see Section 4.2).

$$X_{b,j} = \frac{C_{b,j}}{C_{b,T}}$$

Where $X_{b,j}$ is the concentration fraction of species j in compartment b and $C_{b,T}$ is the sum of species concentrations in compartment b: $\sum X_{b,j} = 1$.

3.2.1 Ionizable Organic Chemicals

For ionizable organic chemicals, the species fractions between neutral and ionic forms can be either provided by the user in the input file of “Chem_Param.xlsx” or calculated in ChemFate using the Henderson-Hasselbalch equations. The equations are dependent on the chemical’s specific pKa and water pH in each compartment. Q_n indicates the fraction of neutral molecules and Q_i indicates the fraction of ions.

$$Q_n = \frac{1}{1 + 10^{\alpha(pH - pKa)}}$$

$$Q_i = 1 - Q_n$$

Where α is 1 for acids and -1 for bases.

3.2.1 Metals

The speciation and partitioning of metals in a water system depends largely on the water characteristics (e.g., pH, ionic strength, temperature, organic matter content). While users need to provide the species fraction values for metals in the input file, those values can be generated from geochemical models such as Visual MINTEQ (Gustafsson, 2017) and WHAM (Centre for Ecology & Hydrology, 2014). Visual MINTEQ is freely available for download to calculate metal partitioning and speciation in the water column, which can be applied to freshwater, marine, sediment pore water, and surface soil water.

For freshwater, marine and sediment pore water, the species fractions in three phases (particulate, colloidal, and dissolved phases) need to be provided by users. The model can then calculate the particulate-to-dissolved partition coefficient (K_{dPD}) and the colloidal-to-dissolved partition coefficient (K_{dCD}). For surface soils, the species fractions in colloidal and dissolved phases also need to be provided by the user, but the particulate phase is optional because ChemFate has several regression models that can estimate the particulate-to-soluble (i.e., dissolved + colloidal) partition coefficient (K_{dPS}) (see Section 3.3.2.3.2). The corresponding K_{dPD} and K_{dCD} is calculated in ChemFate based on the information generated by the geochemical model.

3.3 Phase Distribution Coefficients

The phase partition coefficients are species-specific. In other words, for non-ionizable organic chemicals, only the partition coefficients of the neutral form is required. For non-ionizable organic chemicals, both the neutral form and ionic forms are needed. When available, experimental values from the user are preferred. For metals, the partition coefficients can be calculated provided the user has information on speciation, from experiments or a geochemical model.

3.3.1 Non-ionizable Organic Chemicals

Four partition coefficients are required to run ChemFate - octanol-water partition coefficient (K_{ow} , *unitless*), organic carbon-water partition coefficient (K_{oc} , *L/kg*), air-water partition coefficient (K_{aw} , *unitless*) and aerosol-air partition coefficient

($K_p, m^3/ug$). If experimental values are not available, the partition coefficients can be estimated using EPI Suite (free software provided by the US EPA, 2015).

3.3.1.1 Solid-water partition coefficient (K_d)

There is one additional partition coefficient that is not provided by the user; the solid-water partition coefficient ($K_d, m^3/kg$) is calculated by the model.

$$K_d = K_{oc} \times f_{oc} \times \frac{\rho_{oc}}{1000}$$

Where K_{oc} is organic carbon-water partition coefficient (L/kg), f_{oc} is organic carbon content (kg/kg), ρ_{oc} is solid density (kg/m³), so K_d is solid-water partition coefficient (m³/kg). f_{oc} and ρ_{oc} can be organic carbon in soil, water suspended sediment, and water bottom sediment.

3.3.2. Ionizable Organic Chemicals

When modeling the neutral form of ionizable organic chemicals, the user must provide three partition coefficients - the octanol-water partition coefficient ($K_{ow,n}$, unitless), the organic carbon-water partition coefficient ($K_{oc,n}$, L/kg) and the air-water partition coefficient ($K_{aw,n}$, unitless).

3.3.2.1 Aerosol-air partition coefficient ($K_{p,n}$)

A fourth partition coefficient, the aerosol-air partition coefficient can be provided by the user or calculated by the model. If the $K_{p,n}$ value is unavailable, the user must provide the octanol-air partition coefficient $K_{oa,n}$ which is used to calculate $K_{p,n}$ (Franco and Trapp, 2010; Götz et al., 2007).

$$K_{p,n} = 0.54 \times K_{oa,n} \times f_{oc} \times \frac{\rho_{oc}}{1000}$$

Since ions of ionizable chemicals are assumed nonvolatile, $K_{p,i}$ is 0.

3.3.2.2 Organic carbon-water partition coefficient (K_{oc})

QSAR models can be used to calculate the organic carbon-water partition coefficient ($K_{oc,i}$) of ionizable organic chemicals (Franco and Trapp, 2010; Trapp et al., 2010) in water suspended sediments and sediments. For soil, if the chemical of interest is an organic acid and listed in Table 8, the $K_{oc,i}$ values in the table will be used (Tülp et al., 2009). Otherwise, the $K_{oc,i}$ values will be calculated using the equations below in the model for organic acids and organic bases.

For an organic acid:

$$\text{Log}_{10}K_{ow,i} = \text{Log}K_{ow,n} - 3.5$$

$$K_{ow,apparent} = Q_n \times K_{ow,n} + Q_i \times K_{ow,i}$$

$$K_{oc,i} = pKa^{0.65} \times \left(\frac{K_{ow,apparent}}{K_{ow,apparent} + 1} \right)^{0.14}$$

For an organic base:

$$K_{oc,i} = 10^{(0.11 \times \log(K_{ow,n}) + 1.54)}$$

Table 8. $K_{oc,i}$ values [L/kg] for selected organic acids

Name	CAS	pKa	$K_{oc,i}$
2,4,6-TriCP	88-06-2	6.1	45
2,3,4,6-TeCP	58-90-2	5.4	99
PCP	87-86-5; 6338-69-8	4.8	726
Chloroxynil	1891-95-8	4.9	18
Bromoxynil	1689-84-5	4.3	31
Bromoxynil	1689-84-5	4	46
Ioxynil	1689-83-4	4.5	82
2-NP	79-46-9	7.2	13
4-NP	68081-86-7; 104-40-5; 25154-52-3	7.1	13
2,4-DNP	51-28-5; 1326-82-5; 25550-58-7	3.9	43
Dinoseb	88-85-7	4.6	87
2,4-D	94-75-7; 5742-17-6; 2702-72-9	2.9	21
Mecoprop	93-65-2; 7085-19-0	3.1	11
2,4-DB	94-82-6	5	93
2,4,5-T	93-76-5; 35915-18-5	2.9	48
Ibuprofen	15687-27-1	4.6	12
Ketoprofen	22071-15-4	4.2	17
Fenoprofen	34597-40-5; 29679-58-1; 31879-05-7	4.3	22
Naproxen	26159-31-9; 22204-53-1	4.2	38
Warfarin	81-81-2	5.2	9
Coumachlor	81-82-3	5.2	25

4'-Hydroxywarfarin	24579-14-4	5	9
Coumafuryl	117-52-2	4.3	7
Sulcotrione	99105-77-8; 114680-61-4	2.9	8
Mesotrione	104206-82-8	3.1	8

3.3.2.3 Solid-water partition coefficient (K_d)

3.3.2.3.1 Ionizable Organic Chemicals

Solid-water partition coefficient (K_d) for ionizable organic chemicals in water suspended sediments and sediments are calculated using the organic carbon-water partition coefficient (K_{oc}).

$$K_{d,n} = K_{oc,n} \times f_{oc} \times \frac{\rho_{oc}}{1000}$$

$$K_{d,i} = K_{oc,i} \times f_{oc} \times \frac{\rho_{oc}}{1000}$$

For an organic base in soil, ChemFate uses a cation-exchange model to estimate the sorption of organic cations to soil (Droge and Goss, 2013). The model considers both sorption to organic matter and sorption to phyllosilicate clay minerals.

$$K_{d,i} = K_{CEC,clays} \times (CEC_{soil} - 3.4f_{oc}) + f_{oc} \times D_{oc,IE}$$

$$\log_{10}K_{CEC,clays} = 1.22 \times Vx - 0.22 \times NAI + 1.09$$

$$\log_{10}D_{oc,IE} = 1.53 \times Vx + 0.32 \times NAI - 0.27$$

Where Vx is McGowan's molecular volumes in cm^3/mol and NAI is the number of hydrogens bound by the charged nitrogen. Both molecular descriptors are calculated using Mordred python library (Moriwaki et al., 2018).

3.3.3 Metals

When modeling metals, the solid-water partition coefficient (K_d) must be provided by the user. Once the user generates the species fraction from the chemical speciation model (e.g., Visual MINTEQ), K_{dPD} is calculated by dividing the fraction of chemical sorbed to particulate matter by the fraction of dissolved. K_{dCD} is calculated by dividing the fraction of metals bound to dissolved organic matter to the fraction of dissolved chemical.

$$K_{dPD} = \frac{\text{Fraction of chemical sorbed to particulate matter}}{\text{Fraction of chemical dissolved}}$$

$$K_{dCD} = \frac{\text{Fraction of chemical bound to dissolved organic matter}}{\text{Fraction of chemical dissolved}}$$

When the soil water compositions are not available for the user, K_{dPD} cannot be generated with the chemical species model. Then, ChemFate relies on regression models to calculate K_{dPS} in Table 9 (Sauvé et al., 2000). When the metal in question is not a metal listed in Table 9 and no data are provided, ChemFate uses Cd as a proxy for predicting $K_{d,i}$.

$$\log_{10}(K_{d,i}) = a + b \times pH + c \times \log_{10}(\text{total metal}) + d \times \log_{10}(OM)$$

Where a, b, c, d are coefficients determined using log-based regression models. *Total metal* is the soil metal content in mg/kg and OM is soil organic matter in percentage %.

Table 9. Coefficients for the linear regressions of $K_{d,i}$ for five metals.

Metal	a	b	c	d
Cd	-0.65	0.48	0	0.82
Cu	1.75	0.21	0	0.06
Ni	-4.16	1.02	0	0.80
Pb	1.19	0.37	0.44	0
Zn	-1.34	0.60	0.21	0

3.4 Transport and Transformation Processes

ChemFate dynamically solves for mass transfer between compartments each day. D values are used to quantify the rates of transport and transformation.

For non-ionizable organic chemicals, the mass transport flux (N, mol/day) is calculated as:

$$N = D \times F$$

Where transport D values are in mol/Pa-day and fugacity F is in Pa.

For ionizable organic chemicals, the mass transport flux is calculated as:

$$N = D \times Q$$

Where transport D values are in m³/day and equivalence Q is in mol/m³.

3.4.1 Intermedia Diffusion

Mass transfer across interfaces is modeled using the two-film theory (Reid, 1974). In each phase (e.g. air, water, soil) there is a bulk concentration, which is assumed to be well-mixed and homogeneous, and a boundary layer next to the interface of the other bulk phases with a concentration gradient across the boundary layer. Chemicals transfer

from the bulk phase with a higher concentration to the bulk phase with a lower concentration. Within the boundary layer, diffusive transport is responsible for the movement of molecules from the higher concentration to the lower concentration. The mass transfer coefficients (MTC, m/day) are calculated using the molecular diffusion ($MD_{molecular}$, m²/day) in each phase, and the thickness of each boundary layer (*path length*, in m) for that phase.

$$MTC = \frac{MD_{molecular}}{Path\ length}$$

3.4.1.1 Non-ionizable Organic Chemicals

For non-ionizable organic chemicals, the bi-directional diffusive exchange occurs between air-water, air-soil, and sediment-water phases.

3.4.1.1.1 Air-Water Mass Transfer

The kinetic theory of gases is the most common theoretical approach for calculating molecular diffusivity in the air phase (MD_{air} , in cm²/second). Molecular diffusivity is strongly correlated with the molar volume of the chemical in air (V_{mol} , in m³/mol) (Thibodeaux and Mackay, 2010). The temperature adjustment takes into account of daily fluctuations (T_{daily} , in K) relative to the reference temperature of 25 degree Celsius or 298 K to calculate MD_{air} . The coefficient 8.64 converts the original correlation from cm²/second to m²/day.

$$MD_{air} = 8.64 \times (2.35 \times V_{mol}^{-0.73}) \times \left(\frac{T_{daily}}{T_{ref}} \right)^{1.75}$$

$$MTC_{air} = \frac{MD_{air}}{0.005}$$

The path length for the air boundary is 1 to 10 mm. In ChemFate the default value is 5 mm.

For the water side, ChemFate uses the following equation to estimate the molecular diffusion at dilute concentrations in liquids (Schwarzenbach et al., 2005).

$$MD_{water} = 8.64 \times 0.000274 \times MW^{-0.71}$$

$$MTC_{water} = \frac{MD_{water}}{0.0005}$$

Where MW is molecular mass in g/mol.

The path length for the water boundary is 0.1 to 1 mm. In ChemFate the default value is 0.5 mm.

Since every molecule transferring from the air to water (fresh or marine) or from water to the atmosphere need to pass through two boundary films (air film and water film), the overall mass transfer is a function of the combined effect. $D_{air/water}$ is used to represent the diffusion transport values (mol/Pa-day).

$$D_{air/water} = \frac{1}{\frac{1}{MTC_{air} * A_{A/W} * Z_{air}} + \frac{1}{MTC_{water} * A_{A/W} * Z_{water}}}$$

Where $A_{A/W}$ is the interfacial area between the atmosphere and the corresponding water compartment.

3.4.1.1.2 Air-Soil Mass Transfer

The air side mass transfer coefficient for air-soil mass transfer is the same as the air side mass transfer coefficient for air-water mass transfer, using a default path length of 5 mm.

$$MTC_{air} = \frac{MD_{air}}{0.005}$$

For the chemical mass transfer from soil air to atmosphere, an effective diffusivity in soil air is calculated using the Millington-Quirk equation, with a default path length of 25 mm (Mackay, 2001).

$$MTC_{soil\ air} = \frac{\frac{MD_{air} \times V_{f,soil\ air}^{\frac{10}{3}}}{(V_{f,soil\ air} + V_{f,soil\ water})^2}}{0.025}$$

Where $V_{f,soil\ air}$ and $V_{f,soil\ water}$ are the corresponding soil air and soil water volume fractions. The diffusion path length is 25 mm.

For soil water, a similar approach is taken, with a diffusion path length of 50 mm considered:

$$MTC_{soil\ water} = \frac{\frac{MD_{water} \times V_{f,soil\ water}^{\frac{10}{3}}}{(V_{f,soil\ air} + V_{f,soil\ water})^2}}{0.05}$$

The overall diffusion transport between atmosphere $D_{air/soil}$ (mol/Pa-day) and soil is calculated as follows:

$$D_{air/soil} = \frac{1}{\frac{1}{MTC_{air} \times A_{A/S} \times Z_{air}} + \frac{1}{(MTC_{soil\ air} A_{A/S} \times Z_{air} + MTC_{soil\ water} \times A_{A/S} \times Z_{water})}}$$

Where $A_{A/S}$ is the interfacial area between the atmosphere and the corresponding soil compartment.

3.4.1.1.3 Sediment-Water Mass Transfer

Similarly, the mass transfer between sediment pore water and sediment is calculated as follows, with a default path length of 10 mm (Mackay, 2001):

$$MTC_{sed} = \frac{MD_{water} \times (1 - V_{f,sed solid})^{1.5}}{0.01}$$

Where $V_{f,sed solid}$ is the fraction of solids in the sediment bed.

The overall diffusion transport between sediment and water $D_{sediment/water}$ (mol/Pa-day) is shown below:

$$D_{sediment/water} = \frac{1}{\frac{1}{MTC_{water} \times A_{sed/W} \times Z_{water}} + \frac{1}{MTC_{sed} \times A_{sed/W} \times Z_{sed}}}$$

Where $A_{sed/W}$ is the interfacial area between the water and the corresponding sediment compartment.

3.4.1.2 Ionizable Organic Chemicals

For ionizable organic chemicals, the bi-directional diffusive exchange occurs between air-water, air-soil, and sediment-water phases.

3.4.1.2.1 Air-Water Mass Transfer

The diffusion from air to other compartments (e.g., air and soil air) only occurs for the neutral species, but diffusive transport from water to air occurs for both the neutral and ionic species. ChemFate assumes that the mass transfer coefficient for the neutral and the ionic species are equal (Franco and Trapp, 2010).

$$MTC_{air} = 36 \times (0.3 + 0.2 \times v_{wind}) \times \left(\frac{18}{MW}\right)^{0.335}$$

$$MTC_{water} = 36 \times (0.004 + 0.00004 \times v_{wind}^2) \times \left(\frac{32}{MW}\right)^{0.25}$$

Where v_{wind} is the wind speed (m/second), MW is the molecular weight (g/mol), and MTC_{air} and MTC_{water} are in units of m/hour.

The overall diffusion transport between air and water $D_{Air/Water}$ (m³/day) is shown below:

$$D_{Air/Water} = \frac{1}{\frac{Q_{n,water}}{MTC_{water}} + \frac{1}{MTC_{air,n} \times K_{aw}}} \times \frac{1}{24} \times A_{A/W} \times Z$$

Where $Q_{n,water}$ is the fraction of neutral species in water, K_{aw} is air-water partition coefficient, $A_{A/W}$ is the interfacial area between air and water (m²), Z is the corresponding chemical equivalence capacity (unitless), and the coefficient 1/24 converts hours to days.

3.4.1.2.2 Air-Soil Mass Transfer

For air-soil diffusive transport, only the neutral species diffuses through the air-side boundary layer and soil pore air-side boundary layer. Both the neutral species and ionic species diffuse from the soil water side, and the ion diffusion through the water phase increases the overall transfer process.

$$D_{Air/Soil} = \frac{1}{\frac{1}{\frac{MTC_{soil\ water}}{Q_{n,soil}} + MTC_{soil\ air} \times K_{aw}} + \frac{1}{(MTC_{air} \times K_{aw})}} \times \frac{1}{24} \times A_{A/S} \times Z$$

Where $MTC_{soil\ water}$ is soil water side mass transfer coefficient with value of 2×10^{-6} (m/hour), $MTC_{soil\ air}$ is soil air side mass transfer coefficient with value of 0.02 (m/hour), $Q_{n,soil}$ is the fraction of neutral species in soil pore water, K_{aw} is air-water partition coefficient, $A_{A/S}$ is the interfacial area between air and soil (m²), Z is the corresponding chemical equivalence capacity (unitless).

3.4.1.2.3 Sediment-Water Mass Transfer

Diffusive transport in the water-sediment system transfer between water and sediment pore water for both the neutral and ionic species. The overall diffusion between water and sediment $D_{Water/Sediment}$ (m³/day) is described below:

$$D_{water/sediment} = \frac{1}{\frac{1}{MTC_{water, sed}} + \frac{1}{MTC_{sed\ water}}} \times \frac{1}{24} \times A_{W/Sed} \times Z$$

Where $MTC_{water, sed}$ is water side mass transfer coefficient with value of 0.01 m/hour, and $MTC_{sed\ water}$ is sediment water side mass transfer coefficient with value of 0.0001 m/hour, $A_{W/Sed}$ is the interfacial area between water and sediment (m²), Z is the corresponding chemical equivalence capacity (unitless).

3.4.1.3 Metals

For metals, the bi-directional diffusive exchange only happens between sediment-water phases.

3.4.1.3.1 Sediment-Water Mass Transfer

The water-sediment diffusive exchange for metals applies to colloidal and dissolved metals. The bi-directional diffusion is calculated with an average mass transfer coefficient for the dissolved phase of 1.0×10^{-5} m/h and for the colloidal phase of 7.0×10^{-7} m/h (Bhavsar et al., 2004).

$$D_{water/sediment} = \frac{1}{\frac{1}{MTC_{water,sed}} + \frac{1}{MTC_{sed\ water}}} \times \frac{1}{24} \times A_{W/Sed} \times Z$$

3.4.2 Intermedia Advective Transport

The atmosphere in ChemFate contains two compartments, one representing air and one representing aerosols (a sub-compartment of air). Ionizable and non-ionizable organic chemicals can be suspended in air or can be attached to aerosols. Metals are all assumed to attach to aerosols. ChemFate models multiple advective transport processes including advection in and out of the system, aerosol dry and wet deposition, and rain dissolution.

ChemFate makes distinctions between soil types, including agricultural soils (with or without applied biosolids), urban soils, and undeveloped soils. Within each soil compartment, there are sub-compartment for surface soil, surface soil pore air, surface soil pore water, and a deep soil compartment. The transport processes include surface soil erosion by wind, erosion resulting from water movement, runoff from surface pore water during precipitation events, vertical infiltration from surface soil to deep soil, and horizontal leaching within the deep soil to freshwater. Within soil pore water, ChemFate tracks neutral and ionic species for ionizable organic chemicals and tracks colloidal and ionic species for metals.

ChemFate has two bulk surface water components (generally represented as freshwater and costal marine water). The key transport processes include speciation for ionizable organic chemicals, chemical sorption to suspended sediment, suspended particle sedimentation to water sediment, sediment resuspension, sediment burial to deep sediment, resuspension of free ions to the air in marine costal environments as a result of breaking waves, and advection from freshwater to marine and from marine out of the modeled system as a sink for water, suspended sediment, and sediment.

All the advective transport processes are presented in Table 10. The processes modeled in nanoFate are also showed in Table 10 to give the user a simplified overview of nanoFate. nanoFate tracks three engineered nanomaterial (ENM) states: (1) free nanoparticles and small homoaggregates; (2) ENM particles heteroaggregated with aerosols or suspended sediments; (3) ENM dissolution products in the various waters. Please refer to the nanoFate publication (Garner et al., 2017) for detailed descriptions.

The following sections provide details on each process. Some descriptions are taken from the nanoFate User Guide (Garner et al., 2017) as the calculations for the processes are identical.

Table 10. Key transport and transformation processes in the compartments with tracked chemical forms (i.e., neutral - n, ionic - i) and phases (i.e., dissolved – d, particulate - p, colloidal – c). ENMs means engineered nanomaterials. Symbol “--” means the process is not applicable.

Compartment	Process	organoFate	ionOFate	metalFate	nanoFate
Air	Advection In/Out	n (d, p)	n (d, p), i (d, p)	i (d, p, c)	ENM (i,p)
	Rain Dissolution	n (d)	n (d), i (d)	--	--
	Aerosol Dry Deposition	n (p)	n (p), i (p)	i (d, p)	ENM (i,p)
	Aerosol Wet Deposition	n (p)	n (p), i (p)	i (d, p)	ENM (i,p)
	Air-Water Diffusion	n (d)	n (d), i (d)	--	--
	Air-Soil Diffusion	n (d)	n (d), i (d)	--	--
	Degradation	n (d, p)	n (d, p), i (d, p)	i (d, p, c)	--
	Heteroaggregation	--	--	--	ENM (i,p)
Water	Advection In/Out	n (d, p)	n (d, p), i (d, p)	i (d, p, c)	ENM (i,p)
	Water-Air Diffusion	n (d)	n (d)	--	--
	Suspended Particle Deposition	n (p)	n (p), i (p)	i (p)	ENM (i,p)
	Water-Sediment Diffusion	n (d)	n (d), i (d)	i (d, c)	--
	Aerosol Resuspension	--	--	i (p)	ENM (i,p)
	Dissolution	--	--	--	ENM (d)
Sediment	Advection In/Out	n (d, p)	n (d, p), i (d, p)	i (d, p, c)	ENM (i,p)
	Sediment Resuspension	n (p)	n (p), i (p)	i (p)	ENM (i,p)
	Sediment-Water Diffusion	n (d)	n (d), i (d)	i (d, c)	--
	Burial	n (p)	n (p), i (p)	i (p)	ENM (i,p)
	Dissolution	--	--	--	ENM (d)
Soil	Soil-Air Diffusion	n (d)	n (d), i (d)	--	--
	Runoff (water)	n (d)	n (d), i (d)	i (d, c)	ENM (i,p)
	Erosion (solid)	n (p)	n (p), i (p)	i (p)	ENM (i,p)
	Wind Erosion	n (p)	n (p), i (p)	i (p)	ENM (i,p)
	Soil-Water Partitioning	--	--	--	ENM (i,p)
	Leaching (horizontal)	n (d)	n (d), i (d)	i (d, c)	ENM (i,p)
	Infiltration (vertical)	n (d)	n (d), i (d)	i (d, c)	ENM (i,p)
	Dissolution	--	--	--	ENM (d)

3.4.2.1 Sorption

Sorption is the process of chemicals attaching to solids. Sorption of neutral species and ions is modeled using the solid-water partition coefficient (K_d). ChemFate assumes that an instantaneous equilibrium is reached between water and solid phases based on K_d .

3.4.2.2 Dry Deposition

Dry deposition is the removal of vapors and particulate matter from the atmosphere as a result of gravitational settling, interception, impaction, diffusion, Brownian motion, and turbulence. Stokes' law is used to estimate the deposition velocity of both aerosols and chemicals out of the air compartment. Stokes' Law refers to the velocity at which a spherical object (e.g. a particle) with a small Reynolds number (i.e. very small particles) falls through a fluid. This rate is controlled by a balance between drag force (which keeps the particle suspended) and gravitational force (which is a function of particle size) (Grant et al., 2001). Dry deposition is calculated as:

$$k_{dep} = \frac{2}{9} \times \frac{\rho_p - \rho_a}{\mu} \times g \times R_p^2$$

where k_{dep} is the dry deposition velocity (m/second), ρ_p is the density of the aerosols, ρ_a is the density of the air (kg/m^3), μ is the dynamic viscosity of the air (kg/m-s), g is acceleration due to gravity (m/s^2), and R_p is the radius of either the aerosols.

The transport D value for dry deposition is calculated as.

$$D_{dry\ dep} = k_{dep} \times A_{air/medium} \times V_{f,aer} \times Z_{aero}$$

Where $A_{air/medium}$ is the interfacial area (m^2) between air and receiving compartment, $V_{f,aero}$ is the volume fraction of aerosol in air, Z_{aero} is the Z-value for aerosol.

3.4.2.3 Wet Deposition

Wet deposition is the removal of vapors and particulate matter associated with precipitation (rainfall or snowfall) in the atmosphere by gravitational settling, Brownian, and/or turbulent coagulation with water droplets. The volume fraction of aerosols is calculated accounting for uptake of chemicals. This is then multiplied by the area (m^2), the daily regional precipitation (m/day) and a scavenging ratio of 200,000 (Mackay, 2001), which indicates that a typical single raindrop sweeps through 200,000 times its volume of area.

The transport D value for wet deposition is calculated as.

$$D_{wet\ dep} = k_{rain} \times Scavenging \times A_{air/medium} \times V_{f,aero} \times Z_{aero}$$

Where k_{rain} is rain rate (m/day), *Scavenging* ratio is 200,000 (unitless), $A_{air/medium}$ is the interfacial area between air and receiving compartment (m²), $V_{f,aero}$ is the volume fraction of aerosol in air (unitless), Z_{aero} is the Z-value for aerosol.

3.4.2.4 Advection

Advection is the movement of a chemical resulting from the movement of the medium. In air, the flow rate ($G_{adv,air}$, m³/day) is calculated based on the windspeed (v_{wind} , m/day), the thickness of the atmosphere (h , m), and the area over which the air flows (A m²).

$$G_{adv,air} = v_{wind} \times h \times \sqrt{A}$$

In water, advection is modeled as the transfer from freshwater to coastal marine water for both the water column and suspended sediment, and coastal water out of the modeled system (to open ocean). The flow rate data were collected from the USGS database that provides daily flow estimates (m³/day) for the region. Because no marine flow data is available, ChemFate assumes that the flow rate is the same for both freshwater and marine.

In water sediment, we assume that water column flow causes flow of sediment at 1/10th the rate of water flow, though this rate can be adjusted by the user based on their specific system. This applies to both freshwater, as a transfer from freshwater sediment to marine sediment, and from coastal marine sediment out of the system.

The transport D value for advection is calculated as:

$$D_{adv} = G_{adv} \times Z_{air}$$

3.4.2.5 Wind Erosion

Wind erosion is erosion of the top layer of soil caused by high winds when soil is relatively dry. We use the saltation equation, and the vertical flux conversion to estimate the total transport of soil particles between soil and aerosols and thus the chemicals associated with them (Kelly et al., 2004). Wind erosion is assumed to occur only in undeveloped or agricultural soils because of the general lack of large, open, unpaved or unvegetated spaces in urban areas. It can be estimated using Owen's saltation mass flux, which is given as:

$$Q_{tot} = A \times \frac{\rho}{g} \times \sum_{u_*} u_* \times (u_*^2 - u_{*t}^2) \times \Delta T$$

The saltation mass flux (g/cm-s) is representative of the mass flowing past a pane one length unit wide, perpendicular to both the wind and the ground (Kelly et al., 2004). Q_{tot} is the total horizontal mass flux, A is a dimensionless fitting parameter, generally set to 1 but adjustable to regional variations (Gillette et al., 1997; Webb et al., 2016), ρ is the density of air (kg/m³), g is the acceleration of gravity (m/s²), u_* is the wind shear velocity (m/s), and u_{*t} is the threshold shear velocity (m/s).

Threshold shear velocity is the minimum wind speed necessary to cause erosion of soil particles on the surface (Shao and Lu, 2000). In order to calculate the daily flux of soil particles transported to the air by wind erosion, we first need to know if precipitation occurred recently. If precipitation did occur in the last 24-hours, the minimum threshold shear velocity (u_{*t}) is set to 30 (m/s) because wind erosion is unlikely, though not impossible, when the soil is saturated (this minimum can be altered by the user) (Chepil, 1945). This effect is limited only to the previous day because the effect is generally minimal and temporary. Otherwise, the threshold shear velocity is dependent on the soil texture (Table 11) (Belnap and Gillette, 1998; Gillette and Passi, 1988).

Table 11. Threshold shear velocity by soil type with precipitation.

Surface Soil Texture	Threshold Velocity According to Soil Condition (cm/s)	Threshold Velocity According to Soil Condition when Dry (cm/s)
Sand	25	
Loamy Sand	30	0.533
Sandy Loam	35	0.55
Clay	55	0.716
Silty Clay	55	
Loam	75	
Silt Loam	75	1.416
Clay Loam	75	
Silty Clay Loam	75	
Sandy Clay Loam	75	

Table recreated from Gillette and Passi (1988).

Wind speed for the NOAA data is collected using anemometers situated at 1.5 m above the surface.

$$u_z = \frac{u_*}{k} \times \ln\left(\frac{z}{z_0}\right)$$

The wind shear velocity (u_*) is then calculated from the existing wind speed u_z (m/s) at height z (1.5 m), where k is the von Karmen constant (0.41, unitless), and z_0 is the roughness height (cm) (Sheppard, 1960). The measured wind height (z) must be greater than the roughness height (z_0) or the equation is not valid (Gillette and Passi, 1988; Shao et al., 2009). In simple terms, a larger z_0 would indicate a downward momentum flux, and thus no transfer from soil to air. The roughness height is representative of the roughness of the soil, which has the effect of trapping soil particles and thus limiting the extent of vertical transfer. The roughness value is determined based on the predominant surface coverage of the soil as derived from the Davenport roughness classification (Table 12) (Tufenkji and Elimelech, 2004). These values are representative of the roughness height characteristic of the surface of the soil.

Table 12. Roughness by land cover type.

Surface Cover Type	Roughness (m)
Open Water	0.0002
Open Smooth Terrain	0.0024
Rangeland	0.03
Big Agriculture	0.055
Medium Agriculture	0.1
Orchards	0.2
Suburbs	0.4
Urban	0.6

Taken from Wieringa et al. 1992.

Q_{tot} , calculated two equations prior gives horizontal mass flux. This needs to be converted to vertical mass flux (F_a). A conversion factor (K) is used to convert from horizontal mass flux to the vertical mass flux (F_a , g/cm²-s) (Kelly et al., 2004). F_a is representative of the mass of soil leaving the surface per unit time that remains suspended in the air. The constant, K, reflects the observed linear relationship between F_a and Q_{tot} , which is also based on soil type.

$$F_a = Q_{tot} \times K$$

Table 13. K constant for variations in F_a/Q_{tot} .

Soil Type	K constant (cm ⁻¹)
Clay	10 ^{-6.4}
Loam	10 ^{-5.7}
Sandy Loam	10 ^{-3.7}
Loamy Sand	10 ^{-4.5}
Sand	10 ^{-5.7}

Taken from Gillette et al. 1997 and Kelly et al. 2004.

This equation alone would substantially overpredict transfer from soil to air, so limiting factors are added to account for the large scale of the model and the variability in surface cover. Because wind tends to decrease substantially at night (~10 hrs) and is not consistent throughout the day, we assume that on average for only 5% of that time is there sufficient wind to cause erosion (though both parameters are adjustable within the model) (Chepil, 1945). In addition, this effect is limited to occurring only over that fraction of the soil area that is uncovered due to the absence of any plant material (stubble or weeds or plant matter) that covers the surface of the soil. When vegetation is present it affords substantial protection to the whole soil surface and significantly increases the threshold velocity (Chepil, 1945). In addition, we assume that only 10% of the particles remain in suspension because it is only particles in the dust size range (0.1 – 0.15 mm) that remain in suspension once lifted off the ground by wind (again, this value can be adjusted within the model) (Gillette D.A. and Walker T.R., 1977).

The transport D value for wind erosion is calculated as:

$$D_{windErosion} = \frac{F_a}{\rho_{soil}} \times A_{soil} \times Z_{soilSolid}$$

3.4.2.6 Runoff

Runoff and wet erosion were both modeled using the SCS runoff equation (National Employee Development Center, 1999). Runoff occurs when the rainfall rate exceeds the infiltration rate. The equation is based on the premise that all water that enters and leaves a system is equal. The water balance equation is given as:

$$Q = P - (I_a + F)$$

Where Q is the direct runoff (inches), P is the rainfall (inches/day), I_a is the sum of all losses before the beginning of runoff (inches) and F is the retention after runoff begins (inches). Note that while all input and output units for ChemFate are metric, the SCS equation coefficients were derived from empirical data recorded in the English System of Measurement by the Natural Resource Conservation Service of the United States Department of Agriculture. The necessary metric to English System conversions for model inputs are made internally in ChemFate; the user provides the inputs in the units indicated in the corresponding Region.xlsx spreadsheet. P is provided by the daily precipitation data in the climate data set (“Region.xlsx”, sheet “Climate”). Two assumptions go into estimating I_a and F. The first is that the ratio of the percent water that has been retained to the maximum potential retention is the same as the ratio of the percent water that ran off to the maximum rainfall available for the runoff (Steenhuis et al., 1995).

$$\frac{F}{S} = \frac{Q}{P - I_a}$$

Where F is the amount of rainfall retained (after runoff begins), S is the maximum potential retention (after runoff begins); and $P - I_a$ is the maximum rainfall available for runoff. At the limit where P is exceptionally large, both sides of the equation are essentially equal to 1. When no runoff occurs, both are equal to zero.

The second assumption is that I_a can be expressed as a function of S. NRCS uses the relationship (“Wind Erosion (WEPS) | NRCS,” 2019).

$$I_a = 0.2 \times S$$

Simplifying the equation then results in:

$$Q = \frac{(P - 0.2 \times S)^2}{P + 0.8 \times S}$$

The potential maximum retention after runoff begins has a range of values from 0 to infinity. A more convenient value, known as the curve number (CN) can be used (Soil Conservation Service, 1989).

$$S = \frac{1000}{CN} - 10$$

The transport D value for runoff is calculated as:

$$D_{runoff} = Q \times A_{soil} \times Z_{water}$$

3.4.2.7 Wet Erosion

Soil loss resulting from erosion during precipitation events is calculated using the Revised Universal Soil Loss Equation (RUSLE) (Jones et al., 1996). This equation is commonly used to estimate rates of soil erosion caused by rainfall and the associated overland flow (Lal and Soil and Water Conservation Society (U.S.), 1994). The equation used is:

$$A = R \times K \times LS \times C \times P$$

Where A is the annual soil erosion (tons/ha-year), R is the rainfall-runoff erosivity factor (MJ-mm/ha-h-year), K is the soil erodibility factor (ton-ha-h/ha-MJ-mm), LS is the slope length factor (dimensionless), C is the cover management factor (dimensionless), and P is the support practice factor (dimensionless).

Rainfall-runoff erosivity (R) is a measure of the erosion force caused by rain (Cooper, 2011; Panagos et al., 2015). The R factor is defined as the average annual sum of individual storm erosion index values (EI_{30}), where E is the total storm kinetic energy per unit area, and I_{30} is the maximum 30 minute rainfall intensity (Cooper, 2011). Given the scarce availability of data relating to rainfall intensity, mean annual precipitation is a commonly used alternative (Cooper, 2011; Panagos et al., 2015). Since daily precipitation are available within the model, these values are used to calculate the mean annual precipitation (for each year the model is run), which can then be used to extrapolate the rainfall erosivity factor. The unit rainfall energy (e_r) (MJ/ha-mm) is calculated for each time interval.

$$e_r = 0.29 \times [1 - 0.72 \times e^{-0.05i_r}]$$

where i_r is the rainfall intensity during the time interval (mm/hr) (C. Brown and R. Foster, 1987). Rainfall intensity is replaced by daily precipitation due to data limitations (Panagos et al., 2015). The event erosivity (EI_{30}) is defined as:

$$EI = \left(\sum_{r=1}^0 e_r v_r \right) \times I_{30}$$

where v_r is the rainfall volume (mm) during a time period r , and I_{30} is the maximum rainfall intensity during a 30-minute period of the rainfall event (mm/hr) (Panagos et al., 2015). Thus the R-factor is the product of the kinetic energy of a rainfall event and its maximum 30-minute intensity (C. Brown and R. Foster, 1987).

$$R = \frac{1}{n} \times \sum_{j=1}^n \sum_{k=1}^{mj} (EI_{30})_k$$

Where R is the average annual rainfall erosivity, n is the number of years covered by the data records, and m_j is the number of erosive events of a given year j . Since the model calculates this for each year, there is a correction that allows for partitioning the total rainfall erosivity relative to the amount of precipitation on any given day.

The soil erosivity factor (K) represents the susceptibility of soil to erosion based on the soil texture and composition (Renard et al., 1997; Romkens et al., 1997). These data can be collected from the STATSGO soil dataset (KFFACT) and typically range from 0 to 0.6 (NRCS, 2016). Soils that are high in clay tend to have low K values because they are more resistant to detachment. Coarse textured soils, such as sandy soils, tend to have relatively low K values because of high infiltration relative to runoff even though they are easily detached. Soils with a high silt content tend to have high K values.

The slope length factor (LS) represents the effect of slope steepness and length of field on erosion. Soil loss increases rapidly with slope steepness but is relatively insensitive to slope length (Renard et al., 1997). Because we are dealing with very large areas, the length is set to the maximum value (1000 ft = 304.8 m) and the average slope of each soil region can be calculated from the same STATSGO dataset. (NRCS, 2016) The following conversion is used to determine the LS factor (Table 14).

Table 14. LS factor by slope.

Slope	LS factor with L of 1000 ft
0.2	0.06
0.5	0.1
1	0.2
2	0.47
3	0.8
4	1.19
5	1.63
6	2.11
8	3.15
10	4.56
12	6.28

14	8.11
16	10.02
20	13.99
25	19.13
30	24.31
40	34.48
50	44.02
60	52.7

Taken from Renard et al. 1997 Table 4-2.

The crop management factor (C) is used to reflect the effect of agriculture and management practices on erosion rates (Renard et al., 1997). The C factor is most often used to compare the relative impacts of management options, which is not really the purpose of this model. However, because it can impact the rate of erosion, it also impacts the rate of transfer of chemicals from soil to water. The C-factor is based on the concept of deviation from a standard, in this case a region under clean-tilled continuous-fallow conditions (Renard et al., 1997). C is representative of the effects of plants, soil cover, soil biomass, and activities that may minimize the erosion of soil. For simplicity, we primarily focus on the surface cover, using the NLCD 2011 land cover as a proxy, to estimate the C factor (Table 15).

Table 15. C-factor estimates based on land cover type.

Land Cover	C Factor
Residential and Commercial	0.15
Forest	0.01
Agriculture	0.3
Heterogeneous Crops	0.21
Scrubland	0.05
Barren	0.3
Pasture	0.1

From USDA Publication on estimating sediment loads (Panagos et al. 2015).

The support practice factor (P) reflects the impact of support practices on the average annual erosion rate. It is the ratio of soil loss that occurs with specific practices relative to straight row farming up and-down slope. The P factor differentiates between cropland, rangeland, and permanent pasture and typically ranges from 0 to 1 (with 1 being straight row farming). The lower the value, the better the management practice is at preventing erosion.

Thus total erosion is calculated as:

$$RUSLE = R \times K \times LC \times C \times P$$

ChemFate averages values over very large areas for this calculation, which limits accuracy. This also means that while the variability is probably quite high, there is only one value for soil erosion for each soil type. This value is then calculated over the entire area for each soil type per year and extrapolated to each day based on the daily precipitation relative to the total annual precipitation.

The transport D value for soil erosion is calculated as:

$$D_{erosion} = RUSLE \times \frac{A_{soil}}{\rho_{soil}} \times Z_{soilSolid}$$

3.4.2.8 Vertical Infiltration

Vertical infiltration is the movement of chemicals through the surface soil vertically associated with soil water movement to the deep soil. The daily volume of water infiltrated in mm depends on daily precipitation (mm), soil water runoff (mm), and soil evaporation (mm).

$$Q_{infiltration} = precipitation + runoff - evaporation$$

The soil water volume (m³) is then calculated by:

$$V_{soilwater} = f_{soilwater} \times V_{soil} + Q_{infiltration} \times 0.001 \times A_{soil}$$

Where $f_{soilwater}$ is soil water content with default value of 0.2 and this value can be customized in the Environment file, and 0.001 is used to convert mm to m.

Then, soil field capacity (FC) in m³/m³ is used to determine the soil water infiltration rate in m/day:

$$k_{infiltration} = \frac{FC \times V_{soil} - V_{soilwater}}{A_{soil}}$$

For different soil types, field capacity values can be drawn from Table 16 (Minnesota Pollution Control Agency, 2019).

Table 16. Soil field capacity for different soil types.

Soil	Field Capacity (m ³ /m ³)
Clay	0.32
Clay Loam	0.32
Loam	0.25 to 0.32
Loamy Sand	0.09
Sand	0.17
Sandy Loam	0.14
Silt Loam	0.28
Silty Clay Loam	0.30 to 0.37

The transport D value for leaching is calculated as:

$$D_{leach} = k_{infiltration} \times A_{soil} \times Z_{water}$$

3.4.2.9 Horizontal Leaching

Horizontal leaching is the movement of chemicals through the deep soil horizontally associated with soil water movement to freshwater compartment. The transport D value for horizontal leaching rate is assumed to be the same as vertical infiltration rate (m/day):

$$k_{leaching} = k_{infiltration}$$

$$D_{leaching} = k_{leaching} \times A_{soil} \times Z_{water}$$

3.4.2.10 Sedimentation of Suspended Particulate Matter

Sediment deposition is the process by which suspended particles in water settle to the bottom of a body of water (Mackay, 2001). This settling often occurs when flow slows down or when heavy particles are no longer supported by the innate turbulence of the water. Deposition rates tend to vary from marine to freshwater environments, with much higher rates observed in marine systems (Håkanson, 2006). Deposition of suspended sediment is calculated using Stokes' Law. Settling of suspended sediment is thus calculated as:

$$k_{sed,ss} = \frac{2}{9} \times \frac{\rho_p - \rho_w}{\mu} \times g \times R_p^2$$

where $k_{sed,ss}$ is the flow settling velocity (m/s), ρ_p is the density of the suspended sediment particles (kg/m^3), ρ_w is the density of the water (freshwater or marine for each compartment) (kg/m^3), μ is the dynamic viscosity (kg/m-s), g is acceleration due to gravity (m/s^2), and R_p is the radius of the particles.

The transport D value for suspended particulate matter sedimentation is calculated as:

$$D_{sed,ss} = k_{sed,ss} \times A_{water} \times Z_{water}$$

3.4.2.11 Resuspension of Metals to Aerosols by Coastal Wave Action

Bubble production resulting from oceanic waves breaking in response to sufficiently strong winds allows for transfer of metals in surface marine waters to the aerosols compartment in air (Kerman, 1986). Aerosols from the ocean are formed through bubble formation, followed by bubble collapse and jet ejection, followed by subsequent destabilization to droplets. This process is well established (MACINTYRE, 1970;

MacIntyre, 1968). Bursting bubbles produce two types of droplets: film drops from the rupture of the bubble film, and jet drops by the breakup of the vertically rising jet of water from the collapsing bubble cavity (Blanchard and Woods Hole Oceanographic Institution., 1961; Cipriano and Blanchard, 1981; Thorpe and Barcion, 1982). We primarily focus on the formation and collapse of jet droplets as the mechanism of transfer between surface marine water and aerosols.

For simplicity, we exclude calculations regarding the various sizes of bubbles and assume they are homogeneous and contain the same quantity of chemicals; we assume all bubbles reaching the surface burst allowing for transfer from marine to air (Kerman, 1986). As with soil erosion caused by wind, we again assume that the wind is only sufficiently high for 14 hours out of the day, and of that time period, only 5% of the time is it maintained at sufficient speeds to cause significant aerosol formation.

To compute a representative volume flux (the rate of bubble formation) (V_F) for aerosols with an average diameter of 20 μm at a wind speed of 6 m/s, the commonly used total flux value is 1×10^{-9} cm/s and 9×10^{-4} cm/s for wind speeds greater than 12 m/s (Blanchard and Woods Hole Oceanographic Institution., 1961; Kerman, 1986; Wu et al., 1984). This is then used to calculate the water to aerosols transport ($k_{w,aer}$, m^3/day) relative to the concentration of metals in marine water:

$$k_{w,aer} = EF \times V_F \times A_C$$

where EF is the enrichment factor, V_F is the volume flux (m^3/day), and A_C is the coastal area (m^2) over which this process occurs. This estimate was adapted from a previously completed modeling effort on the transfer of trace metals at the air-water interface (Eisenreich, 1982, 1980; Sievering et al., 1980). The enrichment factor is the metal-to-sodium ratio in the aerosols produced by bubble bursting compared to their ratio in bulk water (Eisenreich, 1980; Hoffman, 1975). This is included because bubbles have been shown to scavenge inorganics from the upper layers of the water (Hoffman, 1975). Enrichment factors are specifically measured for trace metals (Table 16).

Table 17. Enrichment factor for metals.

Metal	Enrichment Factor (Weisel et al. 1984)	Ave. Enrichment Factor (Piotrowicz et al. 1972)	Enrichment Factor (Duce et al. 1975)	Enrichment Factor (Rahn et al. 1975)
Al	200	1.7	0	0
Cd	-	-	730	1200
Co	0.2	-	1.4	5.3
Cr	-	-	10	11
Cu	5	1.1	120	78
Fe	50	1.5	0.4	0.9
Mn	7	0	1.6	4
Pb	8	3.3	2200	800

Sb	-	-	2300	3600
Sc	0.0005	-	-	-
V	10	1.6	16	23
Zn	8	-	110	240

The transport D value for aerosol resuspension is calculated as:

$$D_{aeroResus} = k_{w,aer} \times A_{marine} \times Z_{water}$$

3.4.2.12 Sediment Resuspension

Resuspension is based on the disturbance of the sediment bed by water currents and by biotic activity, which results in transfer back to the suspended sediment compartments. The default rates of resuspension ($k_{sedResusp}$) in the model are given as 3×10^{-7} m³/m²-hr for freshwater and 2×10^{-7} m³/m²-hr for marine and can be modified to be more regionally specific. The area of sediment (A_{sed}) and the Z value for the sediment solid are also accounted for in the calculation.

The transport D value for sediment resuspension is calculated as:

$$D_{sedResusp} = k_{sedResusp} \times A_{sed} \times Z_{sed}$$

3.4.2.13 Burial

Burial is the addition of sediment above existing sediment that “removes” the chemicals from the system. The default rate of burial ($k_{sedBurial}$) for sediments is 4.19×10^{-8} m³/m²-hr for freshwater and 4.5×10^{-8} m³/m²-hr for marine, though these values can be altered by the user to account for regional variations. The area of sediment (A_{sed}) and the Z value for the sediment solid are also accounted for in the calculation.

The transport D value for sediment burial is calculated as:

$$D_{sedBurial} = k_{sedBurial} \times A_{sed} \times Z_{sed}$$

3.4.3 Transformation Processes

ChemFate assumes that the overall reaction process, which is the sum of individual reaction processes, follows a first order reaction process:

$$-\frac{dC}{dt} = k_{deg}C$$

$$C_t = C_0 \times \exp(-k_{deg}t)$$

C is the concentration of the chemical in any given compartment (mol/m³), k_{deg} is the degradation rate constant (day⁻¹), t is time (day), C_0 is the initial concentration, and $C_{(t)}$ is the concentration at any time t. In many instances, predictive tools for overall

transformation process estimate the half-life ($t_{1/2} = HL$, in day). ChemFate converts these half-lives into reaction rate constants.

$$k_{deg} = \frac{\ln(2)}{t_{1/2}}$$

For ionizable organic chemicals, reaction rates are species-specific and they may vary significantly even within a given medium (e.g. air, water). They may also vary spatially, again due to differences in environmental conditions. In Table 18, we provide some general considerations for adjusting the half-life estimates if using EPI Suite for predictions (OCSPP US EPA, 2015). Since metals don't degrade and have little volatility, ChemFate doesn't model degradation for metals.

Table 18. Considerations for adjusting predicted half-lives and reaction rates

Compartment	Reasons for potentially different half-lives
Air phase	
Atmospheric air	Photolysis is one of the most important process for transformation in the atmosphere and may vary based on local solar radiation and length of days. If hydrolysis is an important process, regional variations in air water moisture can also be significant.
Soil pore air	Photolysis can occur on the soil surface, but does not occur in soil pore air, and oxygen content may be lower than in the atmosphere.
Water phase	
Freshwater	Different water chemistries (pH, ions present, redox) can result in different degradation rates. Photolysis in the water column can also be significant
Marine water	
Water in freshwater sediment	Water chemistry, particularly redox, can significantly influence the degradation rates. Photolysis is generally not significant.
Water in marine sediment	
Water in top soil	Biodegradation and hydrolysis are important processes; pH and redox conditions can influence rates significantly. Photolysis does not occur.
Water in deep soil	Low redox conditions are more likely, promoting anaerobic degradation relative to aerobic degradation. Photolysis does not occur.
Solid phase	
Aerosols	In general chemicals sorbed to the solid phase are less available for reacting (e.g. biodegradation, photolysis in aerosols), and thus the reaction rates are much smaller than in the surrounding air or water. Similar considerations for the surrounding air and water are valid (e.g. no photolysis in sediments and soils, pH and redox conditions), in addition to the reduced availability.
Suspended sediments	
Sediment bed solids	
Soil solids	

Degradation constant, calculated from half-life is converted into degradation D-value (m^3/day) as follows:

$$D_{deg,medium} = V_{medium} \times k_{deg,medium} \times Z_{medium}$$

Where V_{medium} is the volume of the subcompartment (m^3) and Z_{medium} is the corresponding Z-value. For non-ionizable organic chemicals, Z value is in unit of $mol/Pa \cdot m^3$, so the D value is in unit of $mol/Pa \cdot day$. For ionizable chemicals, the Z value (unitless) and D value (m^3/day) are both species-specific.

4. Mass Balance Equations

ChemFate keeps track of the chemical movement in a defined region using a series of mass balance equations to solve for the fugacities for non-ionizable organic chemicals and the equivalences for ionizable organics chemicals and metals in each bulk compartment, which is used to calculate the chemical concentrations and mass in the compartment.

Bulk compartments are air (*AirB*), freshwater (*FWB*), freshwater sediment (*FSedB*), marine (*SWB*), marine sediment (*SSedB*), natural soil (*NSB*), deep natural soil (*NSdeepB*), urban soil (*USB*), deep urban soil (*USdeepB*), agricultural soil (*AgSB*), deep agricultural soil (*AgSdeepB*), biosolids agricultural soil (*BioSB*), deep biosolids agricultural soil (*BioSdeepB*).

Sub-compartments are air (Air), freshwater (FW), freshwater suspended sediment (FSS), freshwater sediment water (FSedW), freshwater sediment solids (FSedS), marine (SW), marine suspended sediment (SSS), marine sediment water (SSedW), marine sediment solids (SSedS), soil air (-SA), soil water (-SW), soil solids (-SS).

The transport processes D are denoted as from one compartment to other compartment(s) ($D_{to\ compartment(s)}^{process,from\ compartment}$) or loss from the system ($D^{process,from\ compartment}$). The unit of D for non-ionizable organic chemicals is $mol/Pa \cdot day$ and for ionizable chemicals is m^3/day . N indicates the amount of chemicals released into the system (mol/day), G indicates the advection flow into the system (m^3/day), and C indicates the concentration of the chemicals (mol/kg).

Here is a list of transport and transformation processes and their symbols in the equations.

Process	Symbol
Dry deposition	dryDep
Wet deposition	wetDep
Rain dissolution	rainDiss
Degradation	deg
Advection in	advIn
Advection out	advOut
Diffusion	diffu
Wind erosion	windEro
Resuspension	resusp

Burial	burial
Sedimentation	sed
Soil erosion	erosion
Soil runoff	runoff
Leaching (horizontal)	leach
Infiltration (vertical)	infiltra
Aerosol resuspension	aeroResusp

4.1 Non-ionizable Organic Chemicals

The mass balance equations solving for fugacities of non-ionizable organic chemicals for each bulk compartment are as follows.

For air:

$$V_{AirB} Z_{AirB} \frac{dF_{AirB}}{dt} = -(\sum D_{FWB,SWB,NSB,USB,AgSB,BioSB}^{dryDep,Aero} + \sum D_{FWB,SWB,NSB,USB,AgSB,BioSB}^{wetDep,Aero} + \sum D_{FWB,SWB,NSB,USB,AgSB,BioSB}^{rainDiss,Aero} + \sum D_{FWB,SWB,NSB,USB,AgSB,BioSB}^{diffu,Air} + \sum D_{FWB,SWB,NSB,USB,AgSB,BioSB}^{advOut,Air,Aero} + \sum D_{deg,Air,Aero}) * F_{AirB} + (D_{AirB}^{diffu,FWB} * F_{FWB} + D_{AirB}^{diffu,SWB} * F_{SWB} + D_{AirB}^{diffu,NSB} * F_{NSB} + D_{AirB}^{diffu,USB} * F_{USB} + D_{AirB}^{diffu,AgSB} * F_{AgSB} + D_{AirB}^{diffu,BioSB} * F_{BioSB} + D_{AirB}^{windEro,NSB} * F_{NSB} + D_{AirB}^{windEro,USB} * F_{USB} + D_{AirB}^{windEro,AgSB} * F_{AgSB} + D_{AirB}^{windEro,BioSB} * F_{BioSB} + G_{AirB}^{advIn} * C_{AirB}^{advIn} + N_{AirB})$$

For freshwater:

$$V_{FWB} Z_{FWB} \frac{dF_{FWB}}{dt} = -(D_{AirB}^{diffu,FWB} + D_{FSedB}^{diffu,FWB} + D_{FSedB}^{sed,FSS} + \sum D_{FWB,FW,FSS}^{adv,FW,FSS} + \sum D_{deg,FW,FSS}) * F_{FWB} + [(D_{FWB}^{rainDiss,Aero} + D_{FWB}^{dryDep,Aero} + D_{FWB}^{wetDep,Aero} + D_{FWB}^{diffu,AirB}) * F_{AirB} + (D_{FWB}^{runoff,NSB} + D_{FWB}^{erosion,NSB}) * F_{NSB} + (D_{FWB}^{runoff,USB} + D_{FWB}^{erosion,USB}) * F_{USB} + (D_{FWB}^{runoff,AgS} + D_{FWB}^{erosion,AgS}) * F_{AgSB} + (D_{FWB}^{runoff,BioSB} + D_{FWB}^{erosion,BioSB}) * F_{BioSB} + D_{FWB}^{leach,NSdeepB} * F_{NSdeepB} + D_{FWB}^{leach,USdeepB} * F_{USdeepB} + D_{FWB}^{leach,AgSdeepB} * F_{AgSdeepB} + D_{FWB}^{leach,BioSdeepB} * F_{BioSdeepB} + (D_{FWB}^{diffu,FSedB} + D_{FWB}^{resusp,FSedB}) * F_{FSedB} + G_{FWB}^{advIn} * C_{FWB}^{advIn} + N_{FW} + N_{FSS}]$$

For freshwater sediment:

$$V_{FSedB} Z_{FSedB} \frac{dF_{FSedB}}{dt} = -(D_{FWB}^{diffu,FSedB} + D_{FWB}^{resusp,FSedB} + D_{FSedB}^{burial,FSedS} + \sum D_{FWB,FSedW,FSedS}^{adv,FSedW,FSedS} + \sum D_{deg,FSedW,FSedS}) * F_{FSedB} + [(D_{FSedB}^{diffu,FWB} + D_{FSedB}^{sed,FSS}) * F_{FWB} + G_{FSedB}^{advIn} * C_{FSedB}^{advIn} + N_{FSedB}]$$

For marine:

$$V_{SWB}Z_{SWB} \frac{dF_{SWB}}{dt} = -(D_{AirB}^{diffu,SWB} + D_{SSedB}^{diffu,SWB} + D_{SSedB}^{sed,SSS} + \sum D^{adv,SW,SSS} + \sum D^{deg,SW,SSS}) * F_{SWB} + [(D_{SWB}^{rainDiss,Aero} + D_{SWB}^{dryDep,Aero} + D_{SWB}^{wetDep,Aero} + D_{SWB}^{diffu,AirB}) * F_{AirB} + (D_{SWB}^{diffu,SSedB} + D_{SWB}^{resusp,SSedB}) * F_{SSedB} + \sum D^{adv,FW,FSS} * F_{FWB} + N_{SW} + N_{SSS}]$$

For marine sediment:

$$V_{SSedB}Z_{SSedB} \frac{dF_{SSedB}}{dt} = -(D_{SWB}^{diffu,SSedB} + D_{SWB}^{resusp,SSedB} + D^{burial,SSeds} + \sum D^{adv,SSedW,SSeds} + \sum D^{deg,SSedW,SSeds}) * F_{SSedB} + [(D_{SSedB}^{diffu,SWB} + D_{SSedB}^{sed,SSS}) * F_{SWB} + N_{SSedB}]$$

For natural soil:

$$V_{NSB}Z_{NSB} \frac{dF_{NSB}}{dt} = -(D_{AirB}^{diffu,NSB} + D_{AirB}^{windEro,NSB} + D_{FWB}^{runoff,NSB} + D_{FWB}^{erosion,NSB} + D_{NSdeepB}^{infiltra,NSB} + \sum D^{deg,NSA,NSW,NSS}) * F_{NSB} + [(D_{NSB}^{rainDiss,AirB} + D_{NSB}^{dryDep,AirB} + D_{NSB}^{wetDep,AirB} + D_{NSB}^{diffu,AirB}) * F_{AirB} + N_{NSB}]$$

For deep natural soil:

$$V_{NSdeepB}Z_{NSdeepB} \frac{dF_{NSdeepB}}{dt} = -(D^{deg,NSdeepB} + D_{FWB}^{leach,NSdeepB}) * F_{NSdeepB} + (D_{NSB}^{infiltra,NSB} * F_{NSB} + N_{NSdeepB})$$

For urban soil:

$$V_{USB}Z_{USB} \frac{dF_{USB}}{dt} = -(D_{AirB}^{diffu,USB} + D_{AirB}^{windEro,USB} + D_{FWB}^{runoff,USB} + D_{FWB}^{erosion,USB} + D_{USdeepB}^{infiltra,USB} + \sum D^{deg,USA,USW,USS}) * F_{USB} + [(D_{USB}^{rainDiss,AirB} + D_{USB}^{dryDep,AirB} + D_{USB}^{wetDep,AirB} + D_{USB}^{diffu,AirB}) * F_{AirB} + N_{USB}]$$

For deep urban soil:

$$V_{USdeepB}Z_{USdeepB} \frac{dF_{USdeepB}}{dt} = -(D^{deg,USdeepB} + D_{FWB}^{leach,USdeepB}) * F_{USdeepB} + (D_{USB}^{infiltra,USB} * F_{USB} + N_{USdeepB})$$

For agricultural soil:

$$V_{AgSB}Z_{AgSB}\frac{dF_{AgSB}}{dt} = -(D_{AirB}^{diffu,AgSB} + D_{AirB}^{windEro,AgSB} + D_{FWB}^{runoff,AgSB} + D_{FWB}^{erosion,AgSB} + D_{AgSdeepB}^{infiltra,AgSB} + \sum D_{deg,AgSA,AgSW,AgSS}^{deg,AgSA,AgSW,AgSS}) * F_{AgSB} + (D_{AgSB}^{rainDiss,AirB} + D_{AgSB}^{dryDep,AirB} + D_{AgSB}^{wetDep,AirB} + D_{AgSB}^{diffu,AirB}) * F_{AirB} + N_{AgSB})$$

For deep agricultural soil:

$$V_{AgSdeepB}Z_{AgSdeepB}\frac{dF_{AgSdeepB}}{dt} = -(D_{FWB}^{deg,AgSdeepB} + D_{FWB}^{leach,AgSdeepB}) * F_{AgSdeepB} + (D_{AgSB}^{infiltra,AgSB} * F_{AgSB} + N_{AgSdeepB})$$

For biosolids agricultural soil:

$$V_{BioSB}Z_{BioSB}\frac{dF_{BioSB}}{dt} = -(D_{AirB}^{diffu,BioSB} + D_{AirB}^{windEro,BioSB} + D_{FWB}^{runoff,BioSB} + D_{FWB}^{erosion,BioSB} + D_{BioSdeepB}^{infiltra,BioSB} + \sum D_{deg,BioSA,BioSW,BioSS}^{deg,BioSA,BioSW,BioSS}) * F_{BioSB} + (D_{BioSB}^{rainDiss,AirB} + D_{BioSB}^{dryDep,AirB} + D_{BioSB}^{wetDep,AirB} + D_{BioSB}^{diffu,AirB}) * F_{AirB} + N_{BioSB})$$

For deep biosolids agricultural soil:

$$V_{BioSdeepB}Z_{BioSdeepB}\frac{dF_{BioSdeepB}}{dt} = -(D_{FWB}^{deg,BioSdeepB} + D_{FWB}^{leach,BioSdeepB}) * F_{BioSdeepB} + (D_{BioSB}^{infiltra,BioSB} * F_{BioSB} + N_{BioSdeepB})$$

4.2 Ionizable Chemicals

The construction of mass balance equations for ionizable chemicals is very similar that of non-ionizable chemicals. The two key differences are: 1) the equations are solving for equivalence (Q, mol/m³) instead of fugacity (F, Pa), and 2) neutral and ionic forms are modeled for ionizable organic chemicals, and particulate, colloidal and dissolved phases are modeled for metals in each compartment.

After estimating species-specific Z values (unitless) from species-specific K_d and estimating concentration fractions X (unitless) from species fractions, equivalence fraction Y (unitless) values can be calculated for each bulk compartment. Y_{bj} indicates species j in compartment b.

$$Y_{bj} = \frac{\frac{X_{bj}}{Z_{bj}}}{\sum \left(\frac{X_{bj}}{Z_{bj}} \right)}$$

For ionizable organic chemicals,

$$\begin{aligned} Q_n &= Q * Y_n \\ Q_i &= Q * Y_i \end{aligned}$$

Where Q_n is equivalence of neural form; Q_i is equivalence of ionic form; Q is total equivalence; Y_n is equivalence fraction of neutral form; Y_i is equivalence fraction of ionic form.

For metals:

$$\begin{aligned} Q_p &= Q * Y_p \\ Q_c &= Q * Y_c \\ Q_d &= Q * Y_d \end{aligned}$$

Where Q_p is equivalence of particulate phase; Q_c is equivalence of colloidal phase; Q_d is equivalence of dissolved phase; Q is total equivalence; Y_p is equivalence fraction of particulate phase; Y_c is equivalence fraction of colloidal phase; Y_d is equivalence fraction of dissolved phase.

4.2.1 Ionizable Organic Chemicals

The mass balance equations solving for equivalences of ionizable organic chemicals for each bulk compartment are as follows.

For air:

$$\begin{aligned} V_{AirB} Z_{AirB} \frac{dQ_{AirB}}{dt} = & -[(\sum D_{n,FWB,SWB,NSB,USB,AgSB,BioSB}^{dryDep,Aero} + \sum D_{n,FWB,SWB,NSB,USB,AgSB,BioSB}^{wetDep,Aero} + \sum D_{n,FWB,SWB,NSB,USB,AgSB,BioSB}^{rainDiss,Aero} + \sum D_{n,FWB,SWB,NSB,USB,AgSB,BioSB}^{diffu,Air} + \sum D_n^{advOut,Air,Aero} + \sum D_n^{deg,Air,Aero}) * (Q_{AirB} * Y_{n,AirB}) + (\sum D_{i,FWB,SWB,NSB,USB,AgSB,BioSB}^{dryDep,Aero} + \sum D_{i,FWB,SWB,NSB,USB,AgSB,BioSB}^{wetDep,Aero} + D_i^{advOut,Aero} + D_i^{deg,Aero}) * (Q_{AirB} * Y_{i,AirB})] + [(D_{n,AirB}^{diffu,FWB} * Q_{FWB} * Y_{n,FWB} + D_{n,AirB}^{diffu,SWB} * Q_{SWB} * Y_{n,SWB} + D_{n,AirB}^{diffu,NSB} * Q_{NSB} * Y_{n,NSB} + D_{n,AirB}^{diffu,USB} * Q_{USB} * Y_{n,USB} + D_{n,AirB}^{diffu,AgSB} * Q_{AgSB} * Y_{n,AgSB} + D_{n,AirB}^{diffu,BioSB} * Q_{BioSB} * Y_{n,BioSB} + D_{n,AirB}^{windEro,NSB} * Q_{NSB} * Y_{n,NSB} + D_{n,AirB}^{windEro,USB} * Q_{USB} * Y_{n,USB} + D_{n,AirB}^{windEro,AgSB} * Q_{AgSB} * Y_{n,AgSB} + D_{n,AirB}^{windEro,BioSB} * Q_{BioSB} * Y_{n,BioSB} + D_{i,AirB}^{windEro,NSB} * Q_{NSB} * Y_{i,NSB} + D_{i,AirB}^{windEro,USB} * Q_{USB} * Y_{i,USB} + D_{i,AirB}^{windEro,AgSB} * Q_{AgSB} * Y_{i,AgSB} + D_{i,AirB}^{windEro,BioSB} * Q_{BioSB} * Y_{i,BioSB} + (G_{n,AirB}^{advIn} * C_{n,AirB}^{advIn} + G_{i,AirB}^{advIn} * C_{i,AirB}^{advIn}) + N_{n,AirB} + N_{i,AirB}]) \end{aligned}$$

For freshwater:

$$\begin{aligned}
V_{FWB} Z_{FWB} \frac{dQ_{FWB}}{dt} = & - \left[\left(D_{n,AirB}^{diffu,FWB} + D_{n,FSedB}^{diffu,FWB} + D_{n,FSedB}^{sed,FSS} + \sum D_n^{adv,FW,FSS} \right. \right. \\
& + \left. \sum D_n^{deg,FW,FSS} \right) * (Q_{FWB} * Y_{n,FWB}) \\
& + \left(D_{i,FSedB}^{diffu,FWB} + D_{i,FSedB}^{sed,FSS} + \sum D_i^{adv,FW,FSS} + \sum D_i^{deg,FW,FSS} \right) * (Q_{FWB} \\
& * Y_{i,FWB}) \\
& + \left[(D_{n,FWB}^{rainDiss,Aero} + D_{n,FWB}^{dryDep,Aero} + D_{n,FWB}^{wetDep,Aero} + D_{n,FWB}^{diffu,AirB}) * (Q_{AirB} \right. \\
& * Y_{n,AirB}) + (D_{i,FWB}^{dryDep,Aero} + D_{i,FWB}^{wetDep,Aero} + D_{i,FWB}^{diffu,AirB}) * (Q_{AirB} \\
& * Y_{i,AirB}) + (D_{n,FWB}^{diffu,FSedB} + D_{n,FWB}^{resusp,FSedB}) * Q_{FSed} * Y_{n,FSed} \\
& + (D_{i,FWB}^{diffu,FSedB} + D_{i,FWB}^{resusp,FSedB}) * Q_{FSed} * Y_{i,FSed} \\
& + (D_{n,FWB}^{runoff,NSB} + D_{n,FWB}^{erosion,NSB} + D_{n,FWB}^{leach,NSdeepB}) * Q_{NSB} * Y_{n,NSB} \\
& + (D_{n,FWB}^{runoff,USB} + D_{n,FWB}^{erosion,USB} + D_{n,FWB}^{leach,USdeepB}) * Q_{USB} * Y_{n,USB} \\
& + (D_{n,FWB}^{runoff,AgSB} + D_{n,FWB}^{erosion,AgSB} + D_{n,FWB}^{leach,AgSdeepB}) * Q_{AgSB} * Y_{n,AgSB} \\
& + (D_{n,FWB}^{runoff,BioSB} + D_{n,FWB}^{erosion,BioSB} + D_{n,FWB}^{leach,BioSdeepB}) * Q_{BioSB} * Y_{n,BioSB} \\
& + (D_{i,FWB}^{runoff,NSB} + D_{i,FWB}^{erosion,NSB} + D_{i,FWB}^{leach,NSdeepB}) * Q_{NSB} * Y_{i,NSB} \\
& + (D_{i,FWB}^{runoff,USB} + D_{i,FWB}^{erosion,USB} + D_{i,FWB}^{leach,USdeepB}) * Q_{USB} * Y_{i,USB} \\
& + (D_{i,FWB}^{runoff,AgSB} + D_{i,FWB}^{erosion,AgSB} + D_{i,FWB}^{leach,AgSdeepB}) * Q_{AgSB} * Y_{i,AgSB} \\
& + (D_{i,FWB}^{runoff,BioSB} + D_{i,FWB}^{erosion,BioSB} + D_{i,FWB}^{leach,BioSdeepB}) * Q_{BioSB} \\
& * Y_{i,BioSB} + (G_{n,FWB}^{advIn} * C_{n,FWB}^{advIn} + G_{i,FWB}^{advIn} * C_{i,FWB}^{advIn}) + N_{n,FWB} + N_{i,FWB} \Big]
\end{aligned}$$

For freshwater sediment:

$$\begin{aligned}
V_{FSedB} Z_{FSedB} \frac{dQ_{FSedB}}{dt} = & - \left[(D_{n,FWB}^{diffu,FSedB} + D_{n,FWB}^{resusp,FSedB} + D_n^{burial,FSedS} + \right. \\
& \sum D_n^{adv,FSedW,FSedS} + \sum D_n^{deg,FSedW,FSedS}) * (Q_{FSedB} * Y_{n,FSedB}) + (D_{i,FWB}^{diffu,FSedB} + \\
& D_{i,FWB}^{resusp,FSedB} + D_i^{burial,FSedS} + \sum D_i^{adv,FSedW,FSedS} + \sum D_i^{deg,FSedW,FSedS}) * (Q_{FSedB} * \\
& Y_{i,FSedB}) \Big] + \left[(D_{n,FSedB}^{diffu,FWB} + D_{n,FSedB}^{sed,FSS}) * (Q_{FWB} * Y_{n,FWB}) + D_{i,FSedB}^{diffu,FWB} + D_{i,FSedB}^{sed,FSS} \right) * \\
& (Q_{FWB} * Y_{i,FWB}) + (G_{n,FSedB}^{advIn} * C_{n,FSedB}^{advIn} + G_{i,FSedB}^{advIn} * C_{i,FSedB}^{advIn}) + N_{n,FSedB} + N_{i,FSedB} \Big]
\end{aligned}$$

For marine:

$$\begin{aligned}
V_{SWB}Z_{SWB} \frac{dF_{SWB}}{dt} = & - \left[(D_{n,AirB}^{diffu,SWB} + D_{n,SSedB}^{diffu,SWB} + D_{n,SSedB}^{sed,SSS} + \sum D_n^{adv,SW,SSS} \right. \\
& + \sum D_n^{deg,SW,SSS}) * (Q_{SWB} * Y_{n,SWB}) \\
& + (D_{i,SSedB}^{diffu,SWB} + D_{i,SSedB}^{sed,SSS} + \sum D_i^{adv,SW,SSS} + \sum D_i^{deg,SW,SSS}) * (Q_{SWB} \\
& * Y_{i,SWB}) + [(D_{i,SWB}^{diffu,SSedB} + D_{i,SWB}^{resusp,SSedB}) * (Q_{SSedB} * Y_{i,SSedB}) \\
& + \sum D_n^{adv,FW,FSS} * (Q_{FWB} * Y_{n,FWB}) + \sum D_i^{adv,FW,FSS} * (Q_{FWB} * Y_{i,FWB}) \\
& + N_{n,SWB} + N_{i,SWB}]
\end{aligned}$$

For marine sediment:

$$\begin{aligned}
V_{SSedB}Z_{SSedB} \frac{dQ_{SSedB}}{dt} = & - \left[(D_{n,SWB}^{diffu,SSedB} + D_{n,SWB}^{resusp,SSedB} + D_n^{burial,SSedB} + \right. \\
& \sum D_n^{adv,SSedW,SSedS} + \sum D_n^{deg,SSedW,SSedS}) * (Q_{SSedB} * Y_{n,SSedB}) + (D_{i,SWB}^{diffu,SSedB} + \\
& D_{i,SWB}^{resusp,SSedB} + D_i^{burial,SSedS} + \sum D_i^{adv,SSedW,SSedS} + \sum D_i^{deg,SSedW,SSedS}) * (Q_{SSedB} * \\
& Y_{i,SSedB}) + [(D_{n,SSedB}^{diffu,SWB} + D_{n,SSedB}^{sed,SSS}) * (Q_{SWB} * Y_{n,SWB}) + [(D_{i,SSedB}^{diffu,SWB} + D_{i,SSedB}^{sed,SSS}) * \\
& (Q_{SWB} * Y_{i,SWB}) + N_{n,SSedB} + N_{i,SSedB}]
\end{aligned}$$

For natural soil:

$$\begin{aligned}
V_{NSB}Z_{NSB} \frac{dQ_{NSB}}{dt} = & - \left[(D_{n,AirB}^{diffu,NSB} + D_{n,AirB}^{windEro,NSB} + D_{n,FWB}^{runoff,NSB} + D_{n,FWB}^{erosion,NSB} + \right. \\
& \sum D_n^{deg,NSA,NSW,NSS}) * (Q_{NSB} * Y_{n,NSB}) + (D_{i,AirB}^{windEro,NSB} + D_{i,FWB}^{runoff,NSB} + D_{i,FWB}^{erosion,NSB} + \\
& \sum D_i^{deg,NSA,NSW,NSS}) * (Q_{NSB} * Y_{i,NSB}) + [(D_{n,NSB}^{rainDiss,AirB} + D_{n,NSB}^{dryDep,AirB} + \\
& D_{n,NSB}^{wetDep,AirB} + D_{n,NSB}^{diffu,AirB}) * (Q_{AirB} * Y_{n,AirB}) + (D_{i,NSB}^{dryDep,AirB} + D_{i,NSB}^{wetDep,AirB}) * \\
& (Q_{AirB} * Y_{i,AirB}) + N_{n,NSB} + N_{i,NSB}]
\end{aligned}$$

For deep natural soil:

$$\begin{aligned}
V_{NSdeepB}Z_{NSdeepB} \frac{dQ_{NSdeepB}}{dt} = & - \left[(D_n^{deg,NSdeepB} + D_n^{leach,NSdeepB}) * (Q_{NSdeepB} \right. \\
& * Y_{n,NSdeepB}) + (D_i^{deg,NSdeepB} + D_i^{leach,NSdeepB}) * (Q_{NSdeepB} \\
& * Y_{i,NSdeepB}) + [D_{n,NSB}^{infiltra,NSB} * (Q_{NSB} * Y_{n,NSB}) + D_{i,NSB}^{infiltra,NSB} * (Q_{NSB} \\
& * Y_{i,NSB}) + N_{n,NSdeepB} + N_{i,NSdeepB}]
\end{aligned}$$

For urban soil:

$$\begin{aligned}
V_{USB}Z_{USB} \frac{dQ_{USB}}{dt} = & - \left[(D_{n,AirB}^{diffu,USB} + D_{n,AirB}^{windEro,USB} + D_{n,FWB}^{runoff,USB} + D_{n,FWB}^{erosion,USB} + \right. \\
& \sum D_n^{deg,USA,USW,USS}) * (Q_{USB} * Y_{n,USB}) + (D_{i,AirB}^{windEro,USB} + D_{i,FWB}^{runoff,USB} + D_{i,FWB}^{erosion,USB} +
\end{aligned}$$

$$\sum D_i^{deg,USA,USW,USS}) * (Q_{USB} * Y_{i,USB})] + [(D_{n,USB}^{rainDiss,AirB} + D_{n,USB}^{dryDep,AirB} + D_{n,USB}^{wetDep,AirB} + D_{n,USB}^{diffu,AirB}) * (Q_{AirB} * Y_{n,AirB}) + (D_{i,USB}^{dryDep,AirB} + D_{i,USB}^{wetDep,AirB}) * (Q_{AirB} * Y_{i,AirB}) + N_{n,USB} + N_{i,USB}]$$

For deep urban soil:

$$V_{USdeepB} Z_{USdeepB} \frac{dQ_{USdeepB}}{dt} = -[(D_n^{deg,USdeepB} + D_n^{leach,USdeepB}) * (Q_{USdeepB} * Y_{n,USdeepB}) + (D_i^{deg,USdeepB} + D_i^{leach,USdeepB}) * (Q_{USdeepB} * Y_{i,USdeepB})] + [D_{n,USB}^{infiltra,USB} * (Q_{USB} * Y_{n,USB}) + D_{i,USB}^{infiltra,USB} * (Q_{USB} * Y_{i,USB}) + N_{n,USdeepB} + N_{i,USdeepB}]$$

For agricultural soil:

$$V_{AgSB} Z_{AgSB} \frac{dQ_{AgSB}}{dt} = -[(D_{n,AirB}^{diffu,AgSB} + D_{n,AirB}^{windEro,AgSB} + D_{n,FWB}^{runoff,AgSB} + D_{n,FWB}^{erosion,AgSB} + \sum D_n^{deg,AgSA,AgSW,AgSS}) * (Q_{AgSB} * Y_{n,AgSB}) + (D_{i,AirB}^{windEro,AgSB} + D_{i,FWB}^{runoff,AgSB} + D_{i,FWB}^{erosion,AgSB} + \sum D_i^{deg,AgSA,AgSW,AgSS}) * (Q_{AgSB} * Y_{i,AgSB})] + [(D_{n,AgSB}^{rainDiss,AirB} + D_{n,AgSB}^{dryDep,AirB} + D_{n,AgSB}^{wetDep,AirB} + D_{n,AgSB}^{diffu,AirB}) * (Q_{AirB} * Y_{n,AirB}) + (D_{i,AgSB}^{dryDep,AirB} + D_{i,AgSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{i,AirB}) + N_{n,AgSB} + N_{i,AgSB}]$$

For deep agricultural soil:

$$V_{AgSdeepB} Z_{AgSdeepB} \frac{dQ_{AgSdeepB}}{dt} = -[(D_n^{deg,AgSdeepB} + D_n^{leach,AgSdeepB}) * (Q_{AgSdeepB} * Y_{n,AgSdeepB}) + (D_i^{deg,AgSdeepB} + D_i^{leach,AgSdeepB}) * (Q_{AgSdeepB} * Y_{i,AgSdeepB})] + [D_{n,AgSB}^{infiltra,AgSB} * (Q_{AgSB} * Y_{n,AgSB}) + D_{i,AgSB}^{infiltra,AgSB} * (Q_{AgSB} * Y_{i,AgSB}) + N_{n,AgSdeepB} + N_{i,AgSdeepB}]$$

For biosolids agricultural soil:

$$V_{BioSB} Z_{BioSB} \frac{dQ_{BioSB}}{dt} = -[(D_{n,AirB}^{diffu,BioSB} + D_{n,AirB}^{windEro,BioSB} + D_{n,FWB}^{runoff,BioSB} + D_{n,FWB}^{erosion,BioSB} + \sum D_n^{deg,BioSA,BioSW,BioSS}) * (Q_{BioSB} * Y_{n,BioSB}) + (D_{i,AirB}^{windEro,BioSB} + D_{i,FWB}^{runoff,BioSB} + D_{i,FWB}^{erosion,BioSB} + \sum D_i^{deg,BioSA,BioSW,BioSS}) * (Q_{BioSB} * Y_{i,BioSB})] + [(D_{n,BioSB}^{rainDiss,AirB} + D_{n,BioSB}^{dryDep,AirB} + D_{n,BioSB}^{wetDep,AirB} + D_{n,BioSB}^{diffu,AirB}) * (Q_{AirB} * Y_{n,AirB}) + (D_{i,BioSB}^{dryDep,AirB} + D_{i,BioSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{i,AirB}) + N_{n,BioSB} + N_{i,BioSB}]$$

For deep biosolids agricultural soil:

$$V_{BioSdeepB} Z_{BioSdeepB} \frac{dQ_{BioSdeepB}}{dt} = -[(D_n^{deg,BioSdeepB} + D_n^{leach,BioSdeepB}) * (Q_{BioSdeepB} * Y_{n,BioSdeepB}) + (D_i^{deg,BioSdeepB} + D_i^{leach,BioSdeepB}) * (Q_{BioSdeepB} * Y_{i,BioSdeepB})] + [D_{n,BioSB}^{infiltra,BioSB} * (Q_{BioSB} * Y_{n,BioSB} + D_{i,BioSB}^{infiltra,BioSB} * (Q_{BioSB} * Y_{i,BioSB}) + N_{n,BioSdeepB} + N_{i,BioSdeepB}]$$

4.2.2 Metals

The mass balance equations solving for equivalences of metals for each bulk compartment are as follows.

For air:

$$V_{AirB} Z_{AirB} \frac{dQ_{AirB}}{dt} = -[(\sum D_{p,FWB,SWB,NSB,USB,AgSB,BioSB}^{dryDep,Aero} + \sum D_{p,FWB,SWB,NSB,USB,AgSB,BioSB}^{wetDep,Aero} + D_p^{advOut,Aero}) * (Q_{AirB} * Y_{p,AirB}) + (\sum D_{d,FWB,SWB,NSB,USB,AgSB,BioSB}^{dryDep,Aero} + \sum D_{d,FWB,SWB,NSB,USB,AgSB,BioSB}^{wetDep,Aero} + D_d^{advOut,Aero}) * (Q_{AirB} * Y_{d,AirB}) + D_c^{advOut,Aero} * (Q_{AirB} * Y_{c,AirB})] + [D_{p,AirB}^{windEro,NSB} * (Q_{NSB} * Y_{p,NSB}) + D_{p,AirB}^{windEro,USB} * (Q_{USB} * Y_{p,USB}) + D_{p,AirB}^{windEro,AgSB} * (Q_{AgSB} * Y_{p,AgSB}) + D_{p,AirB}^{windEro,BioSB} * (Q_{BioSB} * Y_{p,BioSB}) + D_{p,SWB}^{aeroResusp,SSS} * (Q_{SWB} * Y_{p,SWB}) + (G_{p,AirB}^{advIn} * C_{p,AirB}^{advIn} + G_{d,AirB}^{advIn} * C_{d,AirB}^{advIn}) + N_{p,AirB} + N_{d,AirB}]$$

For freshwater:

$$\begin{aligned}
V_{FWB} Z_{FWB} \frac{dQ_{FWB}}{dt} = & -[(D_{c,FSedB}^{diffu,FWB} + D_c^{adv,FW}) * (Q_{FWB} * Y_{c,FWB}) \\
& + (D_{d,FSedB}^{diffu,FWB} + D_d^{adv,FW}) * (Q_{FWB} * Y_{d,FWB}) + (D_{p,FSedB}^{sed,FSS} + D_p^{adv,FSS}) \\
& * (Q_{FWB} * Y_{p,FWB})] + [(D_{p,FWB}^{dryDep,Aero} + D_{p,FWB}^{wetDep,Aero}) * (Q_{AirB} * Y_{p,AirB}) \\
& + (D_{d,FWB}^{dryDep,Aero} + D_{d,FWB}^{wetDep,Aero}) * (Q_{AirB} * Y_{d,AirB}) + (D_{c,FWB}^{diffu,FSedB} \\
& * (Q_{FSed} * Y_{c,FSed}) + D_{p,FWB}^{resusp,FSedB} * (Q_{FSed} * Y_{p,FSed}) + D_{d,FWB}^{diffu,FSedB} \\
& * (Q_{FSed} * Y_{d,FSed}) + (D_{c,FWB}^{runoff,NSB} + D_{c,FWB}^{leach,NSdeepB}) * (Q_{NSB} * Y_{c,NSB}) \\
& + (D_{c,FWB}^{runoff,USB} + D_{c,FWB}^{leach,USdeepB}) * (Q_{USB} * Y_{c,USB}) \\
& + (D_{c,FWB}^{runoff,AgSB} + D_{c,FWB}^{leach,AgSdeepB}) * (Q_{AgSB} * Y_{c,AgSB}) \\
& + (D_{c,FWB}^{runoff,BioSB} + D_{c,FWB}^{leach,BioSdeepB}) * (Q_{BioSB} * Y_{c,BioSB}) \\
& + (D_{d,FWB}^{runoff,NSB} + D_{d,FWB}^{erosion,NSB} + D_{d,FWB}^{leach,NSdeepB}) * (Q_{NSB} * Y_{d,NSB}) \\
& + (D_{d,FWB}^{runoff,USB} + D_{d,FWB}^{leach,USdeepB}) * (Q_{USB} * Y_{d,USB}) \\
& + (D_{d,FWB}^{runoff,AgSB} + D_{d,FWB}^{leach,AgSdeepB}) * (Q_{AgSB} * Y_{d,AgSB}) \\
& + (D_{d,FWB}^{runoff,BioSB} + D_{d,FWB}^{leach,BioSdeepB}) * (Q_{BioSB} \\
& * Y_{d,BioSB}) + D_{p,FWB}^{erosion,NSB} * (Q_{NSB} * Y_{p,NSB}) + D_{p,FWB}^{erosion,USB} * (Q_{USB} \\
& * Y_{p,USB}) + D_{p,FWB}^{erosion,AgSB} * (Q_{AgSB} * Y_{p,AgSB}) + D_{p,FWB}^{erosion,BioSB} * (Q_{BioSB} \\
& * Y_{p,BioSB}) + (G_{p,FWB}^{advIn} * C_{p,FWB}^{advIn} + G_{c,FWB}^{advIn} * C_{c,FWB}^{advIn} + G_{d,FWB}^{advIn} * C_{d,FWB}^{advIn}) \\
& + N_{p,FWB} + N_{c,FWB} + N_{d,FWB}]
\end{aligned}$$

For freshwater sediment:

$$\begin{aligned}
V_{FSedB} Z_{FSedB} \frac{dQ_{FSedB}}{dt} = & [-(D_{p,FWB}^{resusp,FSedB} + D_p^{burial,FSedS} + D_p^{adv,FSedS}) * (Q_{FSedB} * \\
& Y_{p,FSedB}) - (D_{d,FWB}^{diffu,FSedB} + D_d^{adv,FSedW}) * (Q_{FSedB} * Y_{d,FSedB}) - (D_{c,FWB}^{diffu,FSedB} + \\
& D_c^{adv,FSedW}) * (Q_{FSedB} * Y_{c,FSedB})] + [D_{c,FWB}^{diffu,FWB} * (Q_{FWB} * Y_{c,FWB}) + D_{d,FWB}^{diffu,FWB} * \\
& (Q_{FWB} * Y_{d,FWB}) + D_{p,FWB}^{sed,FSS} * (Q_{FWB} * Y_{p,FWB}) + G_{p,FWB}^{advIn} * C_{p,FWB}^{advIn} + G_{c,FWB}^{advIn} * \\
& C_{c,FWB}^{advIn} + G_{d,FWB}^{advIn} * C_{d,FWB}^{advIn} + N_{p,FWB} + N_{c,FWB} + N_{d,FWB}]
\end{aligned}$$

For marine:

$$\begin{aligned}
V_{SWB} Z_{SWB} \frac{dQ_{SWB}}{dt} = & [- (D_{p,SSedB}^{sed,SSS} + D_p^{adv,SSS}) * (Q_{SWB} * Y_{p,SWB}) - D_c^{adv,SWB} * (Q_{SWB} \\
& * Y_{c,SWB}) - D_d^{adv,SWB} * (Q_{SWB} * Y_{d,SWB}) - D_{d,SSedB}^{diffu,SWB} * (Q_{SWB} * Y_{d,SWB}) \\
& - D_{c,SSedB}^{diffu,SWB} * (Q_{SWB} * Y_{c,SWB}) - D_{p,AirB}^{aeroResusp,SWB} * (Q_{SWB} * Y_{p,SWB})] \\
& + [(D_{p,SWB}^{dryDep,Aero} + D_{p,SWB}^{wetDep,Aero}) * (Q_{AirB} * Y_{p,AirB}) + (D_{d,SWB}^{dryDep,Aero} \\
& + D_{d,SWB}^{wetDep,Aero}) * (Q_{AirB} * Y_{d,AirB}) + D_{c,SWB}^{diffu,SSedB} * (Q_{SSedB} * Y_{c,SSedB}) \\
& + D_{p,SWB}^{resusp,SSedB} * (Q_{SSedB} * Y_{p,SSedB}) \\
& + D_p^{adv,FSS} * (Q_{FWB} * Y_{p,FWB}) + D_c^{adv,FW} * (Q_{FWB} * Y_{c,FWB}) + D_d^{adv,FW} \\
& * (Q_{FWB} * Y_{d,FWB}) + G_{p,SWB}^{advIn} * C_{p,SWB}^{advIn} + G_{c,SWB}^{advIn} * C_{c,SWB}^{advIn} + G_{d,SWB}^{advIn} * C_{d,SWB}^{advIn} \\
& + N_{p,SWB} + N_{c,SWB} + N_{d,SWB}]
\end{aligned}$$

For marine sediment:

$$\begin{aligned}
V_{SSedB} Z_{SSedB} \frac{dQ_{SSedB}}{dt} = & [- (D_{p,SWB}^{resusp,SSedB} + D_p^{burial,SSeds} + D_p^{adv,SSeds}) * (Q_{SSedB} * Y_{p,SSedB}) \\
& - (D_{d,SWB}^{diffu,SSedB} + D_d^{adv,SSedW}) * (Q_{SSedB} * Y_{d,SSedB}) \\
& - (D_{c,SWB}^{diffu,SSedB} + D_c^{adv,SSedW}) * (Q_{SSedB} * Y_{c,SSedB})] + [D_{c,SSedB}^{diffu,SWB} \\
& * (Q_{SWB} * Y_{c,SWB}) + D_{d,SSedB}^{diffu,SWB} * (Q_{SWB} * Y_{d,SWB}) + D_{p,SSedB}^{sed,SSS} * (Q_{SWB} \\
& * Y_{p,SWB}) + D_{p,SSedB}^{adv,FSedB} * (Q_{FSedB} * Y_{p,FSedB}) + D_{c,SSedB}^{adv,FSedB} * (Q_{FSedB} \\
& * Y_{c,FSedB}) + D_{d,SSedB}^{adv,FSedB} * (Q_{FSedB} * Y_{d,FSedB}) + N_{p,SSedB} + N_{c,SSedB} \\
& + N_{d,SSedB}]
\end{aligned}$$

For natural soil:

$$\begin{aligned}
V_{NSB} Z_{NSB} \frac{dQ_{NSB}}{dt} = & [- (D_{p,AirB}^{windEro,NSB} + D_{p,FWB}^{erosion,NSB}) * (Q_{NSB} * Y_{p,NSB}) - \\
& (D_{d,FWB}^{runoff,NSB} + D_{d,NSdeepB}^{infiltra,NSB}) * (Q_{NSB} * Y_{d,NSB}) - (D_{c,FWB}^{runoff,NSB} + D_{c,NSdeepB}^{infiltra,NSB}) * \\
& (Q_{NSB} * Y_{c,NSB})] + [(D_{p,NSB}^{dryDep,AirB} + D_{p,NSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{p,AirB}) + (D_{d,NSB}^{dryDep,AirB} + \\
& D_{d,NSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{d,AirB}) + N_{p,NSB} + N_{c,NSB} + N_{d,NSB}]
\end{aligned}$$

For deep natural soil:

$$\begin{aligned}
V_{NSdeepB} Z_{NSdeepB} \frac{dQ_{NSdeepB}}{dt} = & [- D_c^{leach,NSdeepB} * Q_{NSdeepB} * Y_{c,NSdeepB} - D_d^{leach,NSdeepB} * Q_{NSdeepB} \\
& * Y_{d,NSdeepB}] + [D_{c,NSB}^{infiltra,NSB} * Q_{NSB} * Y_{c,NSB} + D_{d,NSB}^{infiltra,NSB} * Q_{NSB} \\
& * Y_{d,NSB} + N_{p,NSdeepB} + N_{c,NSdeepB} + N_{d,NSdeepB}]
\end{aligned}$$

For urban soil:

$$V_{USB}Z_{USB}\frac{dQ_{USB}}{dt} = [-(D_{p,AirB}^{windEro,USB} + D_{p,FWB}^{erosion,USB}) * (Q_{USB} * Y_{p,USB}) - (D_{d,FWB}^{runoff,USB} + D_{d,USdeepB}^{infiltra,USB}) * (Q_{USB} * Y_{d,USB}) - (D_{c,FWB}^{runoff,USB} + D_{c,USdeepB}^{infiltra,USB}) * (Q_{USB} * Y_{c,USB})] + [(D_{p,USB}^{dryDep,AirB} + D_{p,USB}^{wetDep,AirB}) * (Q_{AirB} * Y_{p,AirB}) + (D_{d,USB}^{dryDep,AirB} + D_{d,USB}^{wetDep,AirB}) * (Q_{AirB} * Y_{d,AirB}) + N_{p,USB} + N_{c,USB} + N_{d,USB}]$$

For deep urban soil:

$$V_{USdeepB}Z_{USdeepB}\frac{dQ_{USdeepB}}{dt} = [-D_c^{leach,USdeepB} * Q_{USdeepB} * Y_{c,USdeepB} - D_d^{leach,USdeepB} * Q_{USdeepB} * Y_{d,USdeepB}] + [D_{c,USB}^{infiltra,USB} * Q_{USB} * Y_{c,USB} + D_{d,USB}^{infiltra,USB} * Q_{USB} * Y_{d,USB} + N_{p,USdeepB} + N_{c,USdeepB} + N_{d,USdeepB}]$$

For agricultural soil:

$$V_{AgSB}Z_{AgSB}\frac{dQ_{AgSB}}{dt} = [-(D_{p,AirB}^{windEro,AgSB} + D_{p,FWB}^{erosion,AgSB}) * (Q_{AgSB} * Y_{p,AgSB}) - (D_{d,FWB}^{runoff,AgSB} + D_{d,AgSdeepB}^{infiltra,AgSB}) * (Q_{AgSB} * Y_{d,AgSB}) - (D_{c,FWB}^{runoff,AgSB} + D_{c,AgSdeepB}^{infiltra,AgSB}) * (Q_{AgSB} * Y_{c,AgSB})] + [(D_{p,AgSB}^{dryDep,AirB} + D_{p,AgSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{p,AirB}) + (D_{d,AgSB}^{dryDep,AirB} + D_{d,AgSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{d,AirB}) + N_{p,AgSB} + N_{c,AgSB} + N_{d,AgSB}]$$

For deep agricultural soil:

$$V_{AgSdeepB}Z_{AgSdeepB}\frac{dQ_{AgSdeepB}}{dt} = [-D_c^{leach,AgSdeepB} * Q_{AgSdeepB} * Y_{c,AgSdeepB} - D_d^{leach,AgSdeepB} * Q_{AgSdeepB} * Y_{d,AgSdeepB}] + [D_{c,AgSB}^{infiltra,AgSB} * Q_{AgSB} * Y_{c,AgSB} + D_{d,AgSB}^{infiltra,AgSB} * Q_{AgSB} * Y_{d,AgSB} + N_{p,AgSdeepB} + N_{c,AgSdeepB} + N_{d,AgSdeepB}]$$

For biosolids agricultural soil:

$$V_{BioSB}Z_{BioSB}\frac{dQ_{BioSB}}{dt} = [-(D_{p,AirB}^{windEro,BioSB} + D_{p,FWB}^{erosion,BioSB}) * (Q_{BioSB} * Y_{p,BioSB}) - (D_{d,FWB}^{runoff,BioSB} + D_{d,BioSdeepB}^{infiltra,BioSB}) * (Q_{BioSB} * Y_{d,BioSB}) - (D_{c,FWB}^{runoff,BioSB} + D_{c,BioSdeepB}^{infiltra,BioSB}) * (Q_{BioSB} * Y_{c,BioSB})] + [(D_{p,BioSB}^{dryDep,AirB} + D_{p,BioSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{p,AirB}) + (D_{d,BioSB}^{dryDep,AirB} + D_{d,BioSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{d,AirB}) + N_{p,BioSB} + N_{c,BioSB} + N_{d,BioSB}]$$

$$Y_{p,AirB}) + (D_{d,BioSB}^{dryDep,AirB} + D_{d,BioSB}^{wetDep,AirB}) * (Q_{AirB} * Y_{d,AirB}) + N_{p,BioSB} + N_{c,BioSB} + N_{d,BioSB}]$$

For deep biosolids agricultural soil:

$$\begin{aligned} V_{BioSdeepB} Z_{BioSdeepB} \frac{dQ_{BioSdeepB}}{dt} \\ = [-D_c^{leach,BioSdeepB} * Q_{BioSdeepB} * Y_{c,BioSdeepB} - D_d^{leach,BioSdeepB} \\ * Q_{BioSdeepB} * Y_{d,BioSdeepB}] + [D_{c,BioSB}^{infiltra,BioSB} * Q_{BioSB} * Y_{c,BioSB} \\ + D_{d,BioSB}^{infiltra,BioSB} * Q_{BioSB} * Y_{d,BioSB} + N_{p,BioSdeepB} + N_{c,BioSdeepB} \\ + N_{d,BioSdeepB}] \end{aligned}$$

4.3 Solving the Ordinary Differential Equations

ChemFate solves the differential equations on a daily time step because the input parameters like rainfall, wind speed, and release of chemicals are measured on a daily basis. Within Python, the *ode* function from the *scipy.integrate* package is used to solve the equations. The solver takes the value at the end of the day as the solution and use it as the initial condition for the next day. A medium order of 5 is chosen as a general computing engine to approximate the solution of the ordinary differential equations (ODE), because it provides automatic error control that can improve the quality of the computed solutions and lead to relevant savings in computing time (Semplice et al., 2012).

5. Custom Environment Development

This section describes a detailed step-by-step instructions on how to create a customized region with most of the environmental parameters that are required in the input file “Region.xlsx”, sheet “Environment”. The goal is to present the user one option where to find those parameter values, however, the user may find other ways to gather them.

5.1 Create Region of Interest and Download Hydrologic Data in BASINS

We use a publicly available software BASINS(ORD US EPA, 2015), developed by U.S. EPA for water quality-based studies, to identify the region of interest through the selection of watershed(s). Below are the steps to define your region of interest and download hydrologic data:

- 1) Open BASINS v4.5.
- 2) Select “Build New Project”.

- 3) Use the “Select” tool to select your chosen watershed.
 - a. If you are interested in multiple watersheds, you can hold the Ctrl button as you select.
 - b. You can deselect a watershed by clicking on another watershed or holding Ctrl and select the same watershed again.
 - c. Write down the HUC (hydrologic unit code) number of your selected watershed(s) (you will use it when you download STORET data later for water quality information).
 - d. Click on “Build” button.
- 4) Set projection properties for your interested region.
 - a. Set Category to UTM-1983.
 - b. Search the UTM zone(s) through the link:
<http://www.dmap.co.uk/utmworld.htm>
- 5) Download additional basic data for your interested region. The downloaded data will be processed in the next session in GIS software.
 - a. Select “File”, then select “Download Data”.
 - b. Set “Region to Download” to “Hydrologic Units”.
 - c. Download each of the following data types at a time, check the boxes “Merge” and “Clip to Region”. Click on “Save” after each download.
 - i. DEM grid (Digital Elevation Model), and check watershed outflows
 - ii. NHD (National Hydrography Dataset)
- 6) River depth calculation.
 - a. Open “rf1.bdf” in excel, and calculated weighted average depth (column “PDEPTH”) based on length (column “LENGTH”).

5.2 Soil Data Preprocessing using GIS

Here, we use Esri ArcGIS to process the data, but you can also use other GIS tools. From BASINS software, we have downloaded statsgo soil data that contains many soil attributes (e.g., organic carbon content, erodibility factor, slope).

- 1) Open ArcGIS.
- 2) Select “add data” and add the folder of your region created in BASINS.
- 3) Select 4 files to display on the “Table of Contents”
 - a. “cat.shp”
 - b. “statsgo.shp”
 - c. “statsgoc.dbf”
 - d. “statsgol.dbf”
- 4) Dissolve “cat.shp” file into one single file by selecting “geoprocessing” and then selecting “dissolve”.
 - a. Input Features: cat
 - b. Output Feature Class:

- i. Go to the BASINS data folder.
 - ii. Create a new folder “regional_data”.
 - iii. Save it as “regional_boundary”.
- 5) Join “statsgo.shp” with “statsgoc.dbf” and “statsgol.dbf”.
 - a. Right click on “statsgo” and select “Open Attribute Table”, and you should see the 5th column is MUID.
 - b. Right click on “statsgo” and select “Joins and Relates”, and then select “Join”.
 - i. Choose “Join Attribute from Table”.
 - ii. For 1 choose “MUID” from the dropdown menu.
 - iii. For 2 choose “statsgoc” from the dropdown menu.
 - iv. For 3 choose “MUID” from the dropdown menu.
 - v. For “Join Options”, select “Keep All Records”.
 - vi. Click “Ok” and then “Yes”.
 - c. Repeat the above step to join “statsgol.dbf” to “statsgo.shp”.
- 6) Export “statsgo.shp” to save the file with all those joined data.
 - a. Right click on “statsgo.shp”, and select “Data”, and then select “Export Data”.
 - b. Find the saved BASINS folder.
 - c. Rename to “soil_region.shp”.
 - d. Click “Save”, and then “OK”, and then “Yes”.
- 7) Clip the soil to your interested region:
 - a. Go to “geoprocessing” and select “clip”.
 - i. Input Features: “soil_region.shp”
 - ii. Clip Features: “regional_boundary.shp”
 - iii. Output Feature Class: “soil_clipped.shp”
 - iv. Click “OK”

5.3 NLCD Data Preprocessing using GIS

The National Land Cover Database (NLCD) provides data on land cover at a 30m resolution. We will use this database to classify our interested region into 3 different soil types - national, urban, agriculture. The fourth soil type - agricultural biosoids – depends on the local biosoids application practice.

- 1) Download NLCD Land Cover database: <https://www.mrlc.gov/data>
- 2) Import the NLCD data layer to the ArcGIS.
- 3) Clip the NLCD land cover data by going to “data management tools”, and select “raster”, and select “raster processing”, and select “clip”.
 - a. Input Raster: “nlcd_layer.tif”
 - b. Output Extent: “regional_boundary.shp”
 - c. Output Raster Dataset: go to “regional_data” folder, rename the file to “region_nlcd.tif”

- d. Click “OK”
- 4) Convert raster to shapefile by going to “Toolbox”, and select “conversion tools”, and select “from raster”, and select “Raster to Polygon”.
 - a. Input raster: “region_nlcd.tif”
 - b. Output polygon features: “region_nlcd.shp”
 - c. Unselect “Simplify polygons”
 - d. Click “OK”
- 5) Clip the shapefile to the interested region by going to “geoprocessing”, and select “clip”:
 - a. Input features: “region_nlcd.shp”
 - b. Clip feature: “regional_boundary.shp”
 - c. Output feature class: “region_nlcd_region.shp”
 - d. Click “OK”
- 6) Spatial Join the soil parameters to the interested region by going to “spatial join”, and select “Spatial Join (Analysis)”:
 - a. Target features: “region_nlcd_region.shp”
 - b. Join features: “soil_clipped.shp”
 - c. Output feature class: rename “region_nlcd_soil.shp”
 - d. Select Join Operation “Join One to One”
 - e. Match option “Intersect”
 - f. Select “Keep All Target Features”
 - g. Click “OK”

5.4 Soil Data Processing

- 1) In ArcGIS, right click on “region_nlcd_soil.shp” and select “Open attribute table”.
 - a) Select “add field”
 - b) Name “AREA_grid”, double digits
 - c) Right click on the “AREA_grid”, and select “calculate geometry: area, sqm”
- 2) Open “region_nlcd_soil.dbf” in excel, save as “soil_landuse_processing.xlsx” to do calculations.
- 3) Create a pivot table for the data in “soil_landuse_processing.xlsx”.
 - a) Select “insert”, and then select “pivot table”, and then select “OK”.
- 4) Soil slope calculation from column “SLOPEL” and column “SLOPEH”. We want to calculate the weighted average of soil slopes based on soil types. “SLOPEL” means low soil slope and “SLOPEH” means high soil slope.
 - a) Select “GridCODE” to COLUMNS, “SLOPEL” to ROWS, “AREA_grid” to VALUES (sum).

- b) Open: <https://www.mrlc.gov/data/legends/national-land-cover-database-2011-nlcd2011-legend>
- c) Average slope over each land cover type (classification code 11-95 in column “GridCODE”) using the equation: slope type (%) * area / total_area.
 - i) Do the calculation for “SLOPEL” and “SLOPEH” separately, and average the values.
 - ii) Across each land cover type.
 - iii) Freshwater area is GridCODE 11.
- 5) Soil wet depth calculation from column “WTDEPL” and column “WTDEPH”.
 - a) Do the similar steps as in step 4, except for “WTDEPH” to ROWS.
 - b) Convert depth unit from ft to m by multiplying the conversion factor of 0.3048.
- 6) Soil texture calculation from column “SURFTEX”.
 - a) Create a pivot table with “SURFTEX” to COLUMNS, “GridCODE” to ROWS, and “Area_grid” to VALUES (sum).
 - b) For each soil type, find the largest area of the soil texture.
 - c) Aggregated the soil texture for natural, urban, and agricultural based on the most common texture.
- 7) Soil erodibility calculation from column “KFFACT”.
 - a) Do the similar steps as in step 4, except for “KFFACT” to ROWS.
- 8) Organic carbon calculation from column “OML” and column “OMH”.
 - a) Do the similar steps as in step 4, except for “OML” or “OMH” to ROWS.
- 9) pH calculation from column “PHL” and column “PHH”.
 - a) Do the similar steps as in step 4, except for “PHL” or “PHH” to ROWS.

5.5 Hydrologic Flow Data Collection

- 1) Based on the HUC number (s) of your interested region, go to the USGS website for surface-water data for the nation: <http://waterdata.usgs.gov/nwis/sw>
- 2) Select “Daily Data”.
- 3) Set the “Site Location” to “State/Territory”, and then click “Submit”
- 4) Set “State/Territory” to the state where your interested region belongs to.
- 5) Set “Site Type” to “Lake and Stream”.
- 6) Set “Available Parameters” to “Streamflow, ft³/s”.
- 7) Set “Choose Output Format”:
 - a. Select “Table of sites grouped by Hydrologic Unit”.
 - b. Set “Retrieve data” for the range of simulation time your are interested in, for example from 2005-01-01 to 2014-12-31.
- 8) Search for the downstream HUC number(s) identified before. Here, we use the data from the downstream to be representative of the region’s water flow.

- 9) Open each site in a new tab to see if they provide the data. For those that have data, you can change the dropdown menu to “Location Map”. Choose a site that is the closest to the coastal zone or closest to the outflow point.
- 10) For this site, retrieve data from “Time-series: Daily data”.
 - a. Set “Available Parameters Discharge” to “Mean”.
 - b. Check the “Begin date/End date” to your ideal time period.
 - c. Set “Output” format to “Tab-separated”.
 - d. Click “go” to download the data.
- 11) Save the data by right click and select “Save Page As” a “*.txt” file (* here indicate a file name you entered).
- 12) Open *.txt file in excel and delete all unnecessary rows and columns:
 - a. We only need the dates and flow data.
 - b. Convert the flow data from ft³/s to m³/s by multiplying the conversion factor of 0.0283.
 - c. For some negative values, change it to 0 (more likely in coastal zone).

5.6 Water Quality Data STORET Collection

- 1) Go to the website: www3.epa.gov/storet
- 2) Click on “Get Data”.
- 3) Click on “Download STORET Data”.
https://ofmpub.epa.gov/storpubl/dw_pages.querycriteria
- 4) Go to “select one or more drainage basin/HUC” and click on “Look Up and search” for the HUCs for your region of interest.
- 5) Set “Station type” to “River/Stream and Lake” for freshwater and “Ocean” for marine water.
- 6) Set “Date” from year you are interested in. If they don’t have data, go back to earlier years. If they still don’t have data, collect data from surrounding regions (HUCs);
- 7) Set “Activity Medium” to “Water”.
- 8) Set “Characteristic Search” to “Suspended Sediment Concentration & Sediment Depth”
- 9) Click “Results Download”.
- 10) In the section of Batch Processing:
 - a. Select the appropriate user profile: University/College
 - b. Enter your email address and file names.
- 11) Select “Immediate”.
- 12) Go back to download the sediment data.
 - a. Set “Activity Medium” to “Sediment”.
 - b. Click “Result download”.
- 13) You should receive two emails, the first saying that they are processing your request and the second with a zip file of the data.

- 14) The COMPLETED email will contain your zip file to download. Extract the files from the zip folder.
- 15) Unzip the file and open the “*RegResults.txt” file in excel.
- 16) Create a pivot table in excel with “Characteristic Name” to ROWS, “Units” to COLUMNS, and “Result Value as Number” to VALUES (average).
- 17) Look for pH average value (from the grand total column in pivot table).
- 18) Look for organic carbon (or carbon, total organic) average value.
 - a. Check the units for multiple values to make sure they are consistent. Otherwise, you need to do the unit conversion.
- 19) Look for Suspended Sediment Concentration average value.
 - a. If the sediment file doesn’t have data, we assume it’s the same as the water above it.
- 20) Look for Sediment Depth average value.

5.7 Marine Environment Buffer Zone

- 1) Open ArcGIS.
- 2) Open “region_boundary.shp” (it should be already dissolved into one shapefile cat).
- 3) In the tool Search box, search for “Polygon to line (conversion)”:
 - a. Input feature: “region_boundary.shp”
 - b. Output feature: in “regional_data” folder, named it “region_outline.shp”
 - c. Select “optional option”
 - d. Click “OK”
- 2) Open Editor to draw the buffer zone.
 - a. Click “start editing”
 - b. Select the outline and split line
 - c. Select two points that distinct the ocean line
 - d. Select the right polyline of ocean
 - e. Click save edits
 - f. Click stop editing
- 3) Output the shape file.
 - a. Right click on “region_outline” and select “Open attribute table”
 - b. Select the coastline (turn green on map)
 - c. Select “Data” and “Export Data”
 - d. Save as “region_coast” and select shape file
- 4) Create the buffer coast line.
 - a. 1000 meters for marine area
 - b. Click on “Geoprocessing” and then select “Buffer”
 - i. Input feature: “region_coast.shp”
 - ii. Linear unit: 1000 meters
 - iii. Side type: LEFT or RIGHT (depends on the region)

- iv. End type: FLAT
- 5) Calculate the area.
 - a. Right click the shape file and select “Open attribute table”.
 - b. Select “Add field”
 - i. Name “Area”, type “double”, unit “sq meter”.
 - c. Right click “Area” column, and select “Calculate geometry”.

5.8 Climate Data Collection

- 1) Go to the NOAA NNDC climate data website to download the data:
<https://www7.ncdc.noaa.gov/CDO/cdoselect.cmd?datasetabbv=GSOD&countryabbv=&georegionabbv=>

- a. Click “I Agree to These Terms”.
- b. Select “County (US)” and then click “Continue”.
- c. Selected “US stations” and then select the state name.
- d. Choose the station name of your region of interest.
- e. Enter the date range of your interest.
- f. Right click on “save page as” and save the “*.txt” file.

This dataset contains daily climatic data of temperature (TEMP, in Fahrenheit), precipitation (PRCP, in inches), wind speed (WSPD, in knots). You need to convert temperature unit to Celsius, precipitation unit to millimeter (mm), wind speed to m/second.

- 2) Evaporation data is from TerraClimate and can be downloaded using an R package called climateR. Since this data is available by month, we assume the same daily evaporation rate within a month.

- a. climateR website: <https://github.com/mikejohnson51/climateR>
- b. R code below is an example of Visalia, Tulare from 2005 to 2014.


```
devtools::install_github("mikejohnson51/climateR")
devtools::install_github("mikejohnson51/AOI")
library(AOI)
library(climateR)
library(sf)
library(devtools)
install_github("r-spatial/sf")
library(sf)
library(raster) # for cellStats

# show parameter name, description and units
param_meta$terraclim # monthly

# get Evapotranspiration data from climateR
params = 'aet' # actual evapotranspiration in mm
# boundary box of visalia, lat (minute to degree), long, box height and
weight in miles
AOI = getAOI(clip=list(36.32, 119.3, 7, 7))
```

```

r = getAOI(clip=list(36.32, 119.3, 7, 7)) %>% getTerraClim(param='aet',
startDate='2005-01-01', endDate='2014-12-31')
# r2 = getAOI(state = 'CA', county='Tulare') %>%
getTerraClim(param='aet', startDate='2005-01-01', endDate='2014-12-31')
data = cellStats(r[[1]], stat = 'mean', na.rm=TRUE)
write.csv(data, "aet_visalia.csv")

```

5.9 Aerosol Data Collection

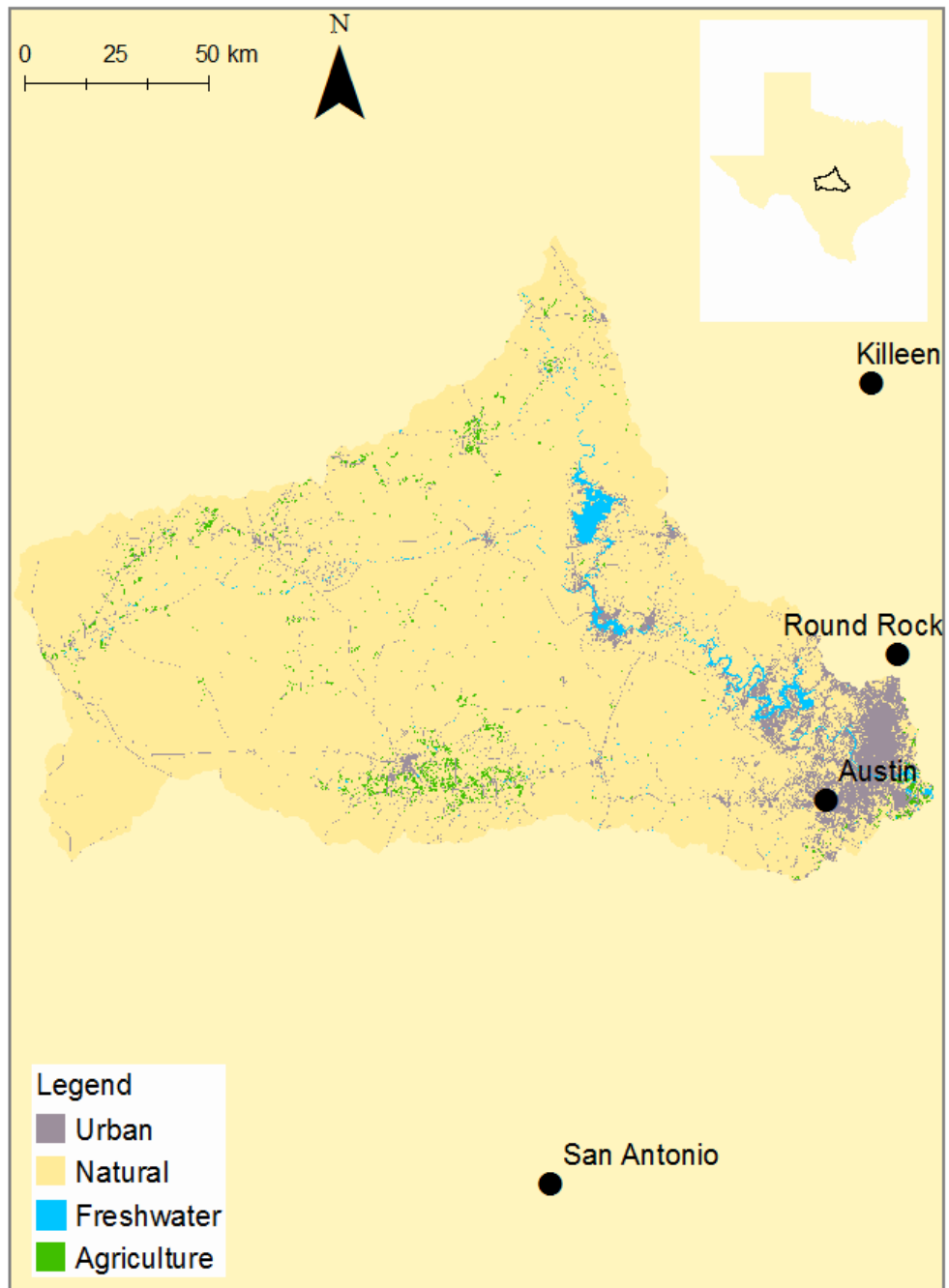
- 1) Go to U.S. EPA air data page and download daily summary data (PM10 Mass 81102): https://aqs.epa.gov/aqsweb/airdata/download_files.html
- 2) Unzip it and save it in the “regional_data” folder.
- 3) Open the excel file and find the aerosol values for your interested region.

6. Appendix I

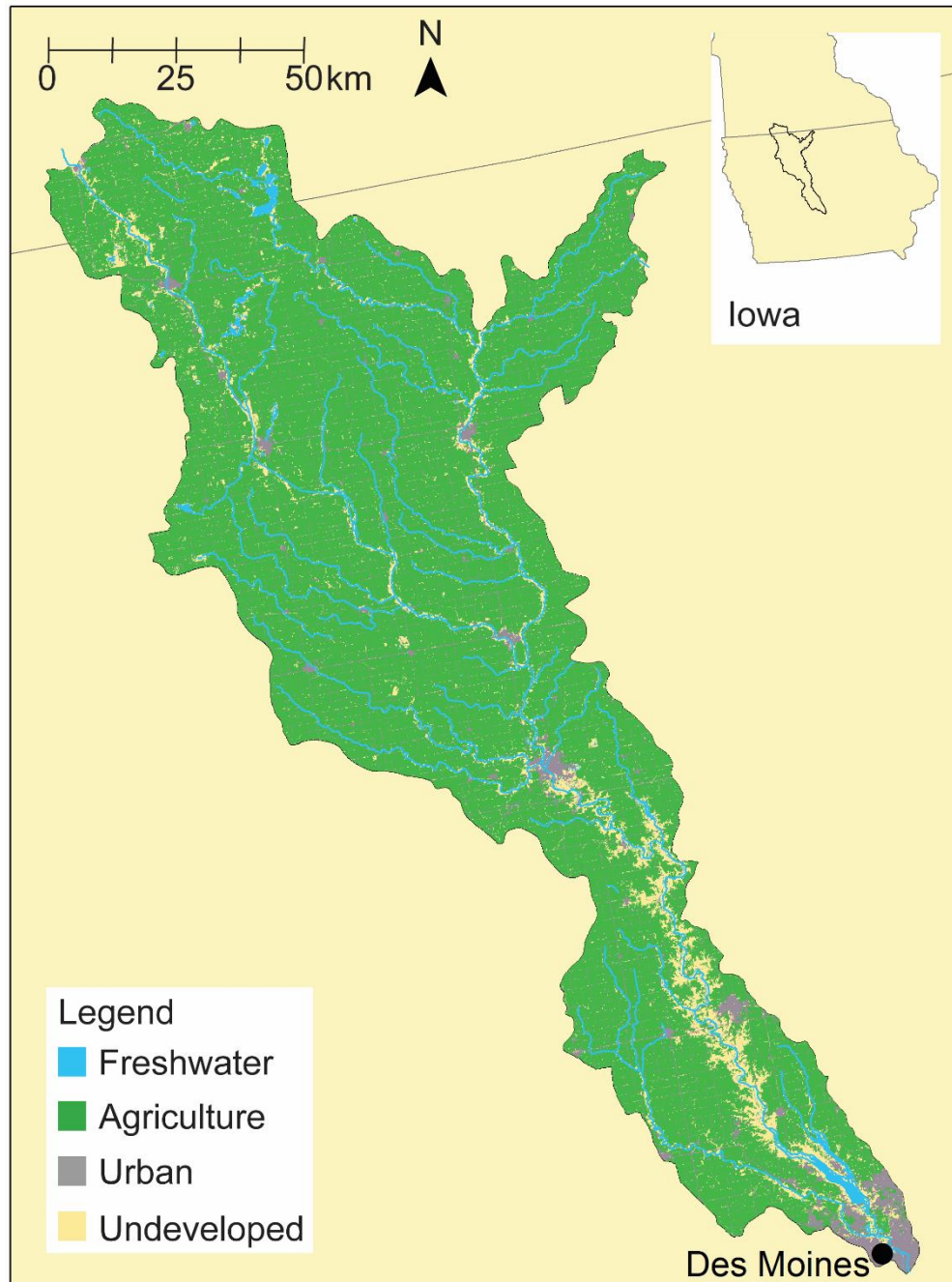
Appendix I

The eight U.S. environments and one global environment were developed by Dr. Kendra Garner, Dr. Mengya Tao, and Yiting Ju. The four European environments were developed by Peter Page, Nicol Parker, and Dr. Kendra Garner.

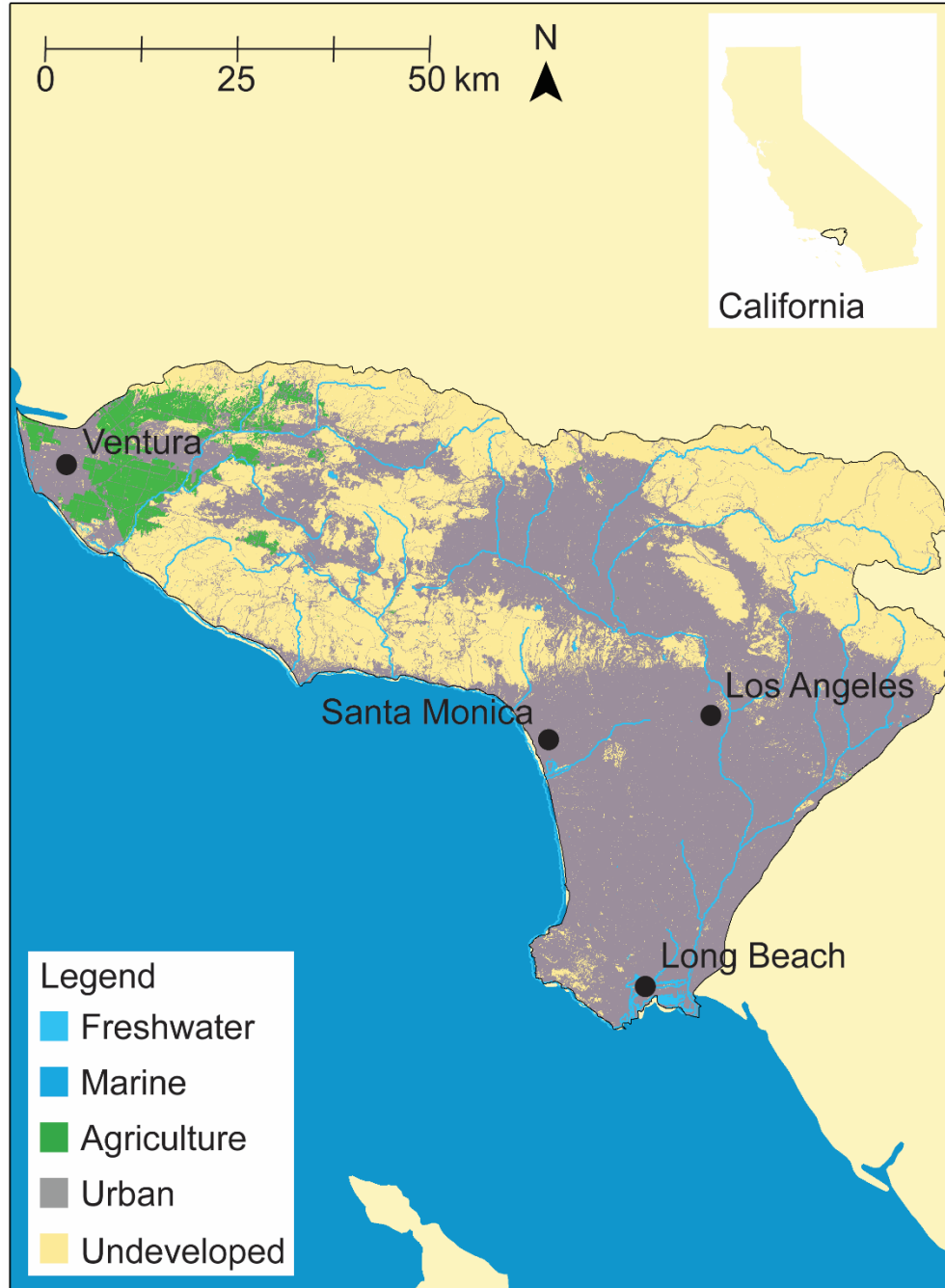
Austin, Texas



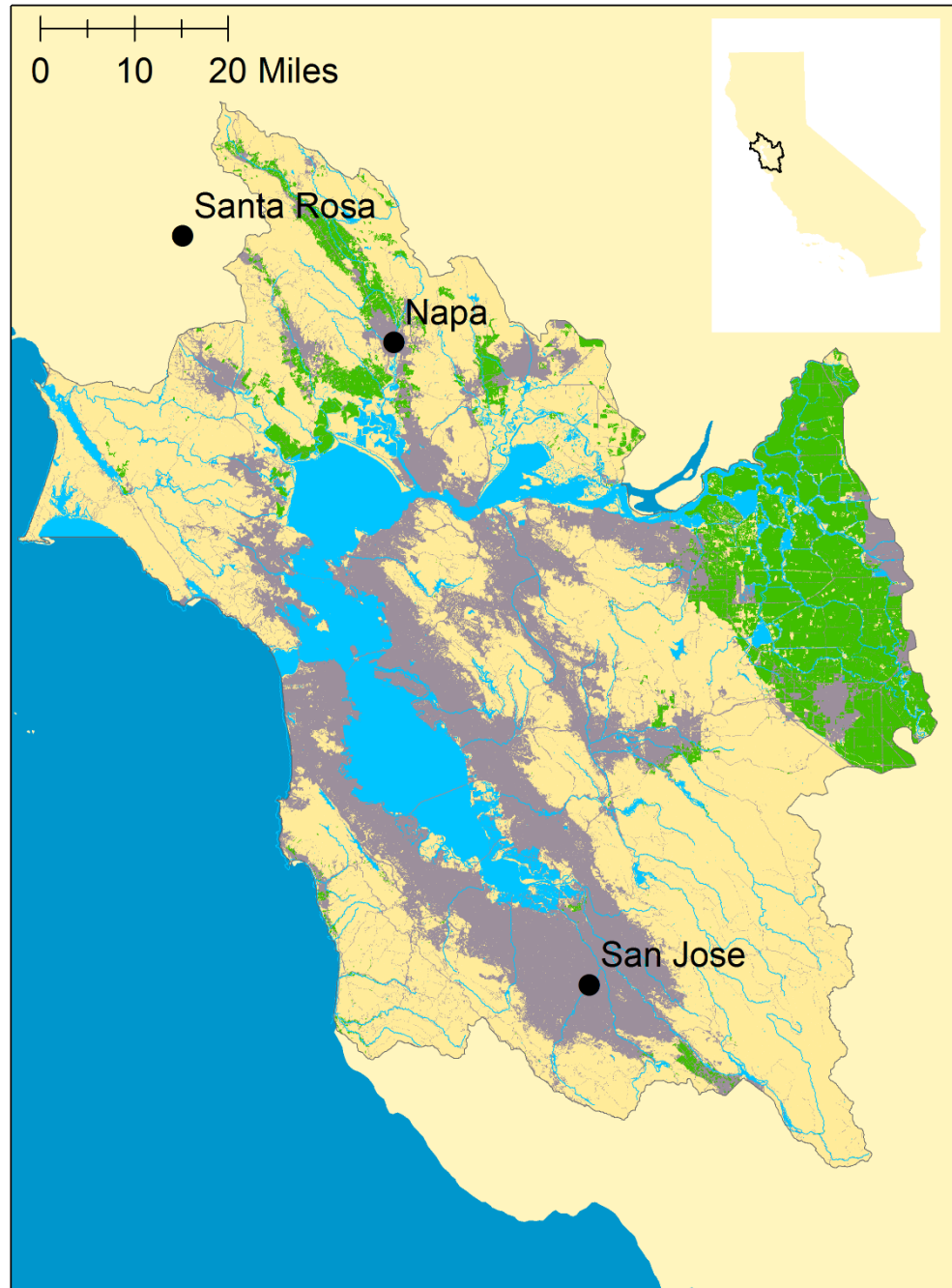
Des Moines, Iowa



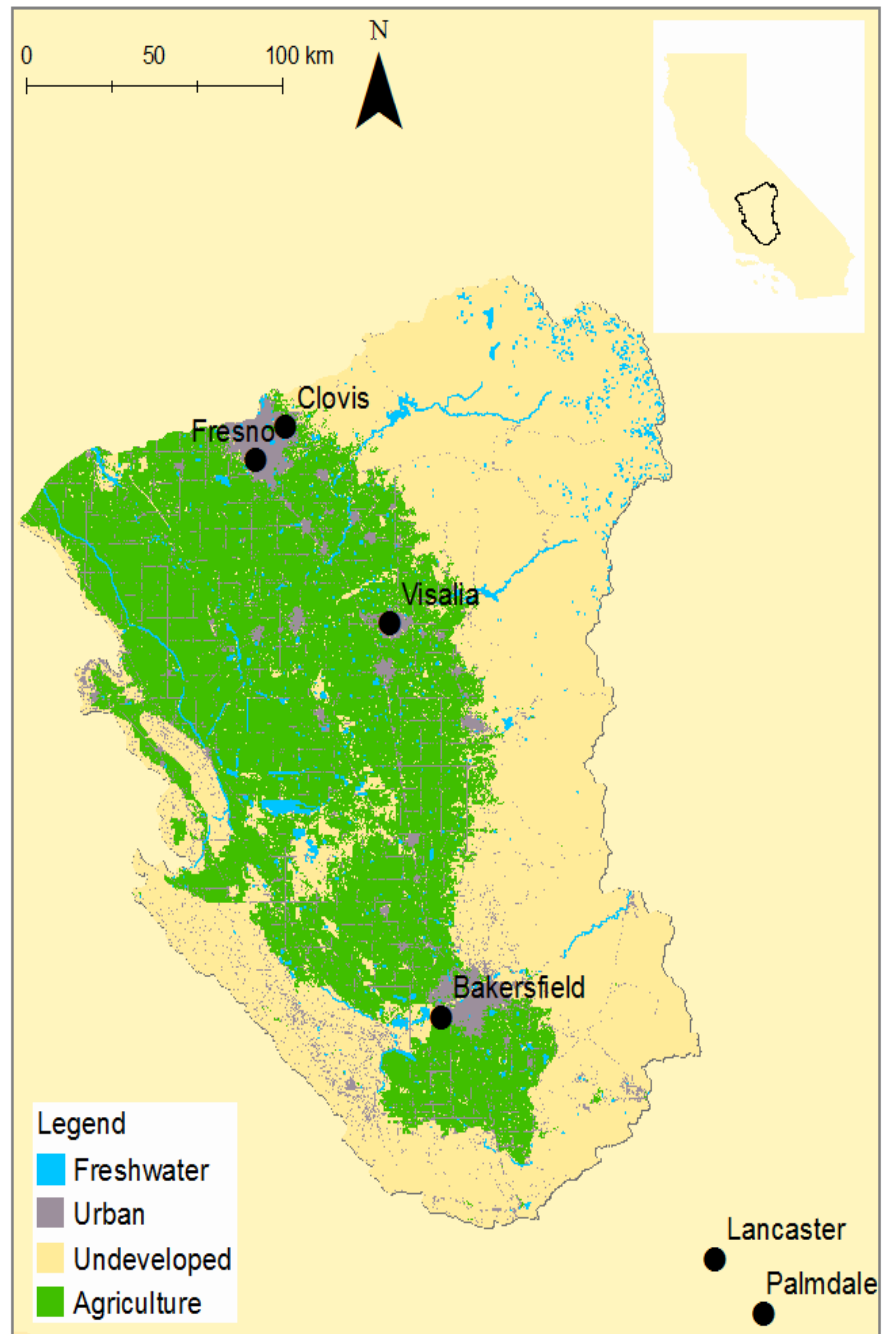
Los Angeles, California



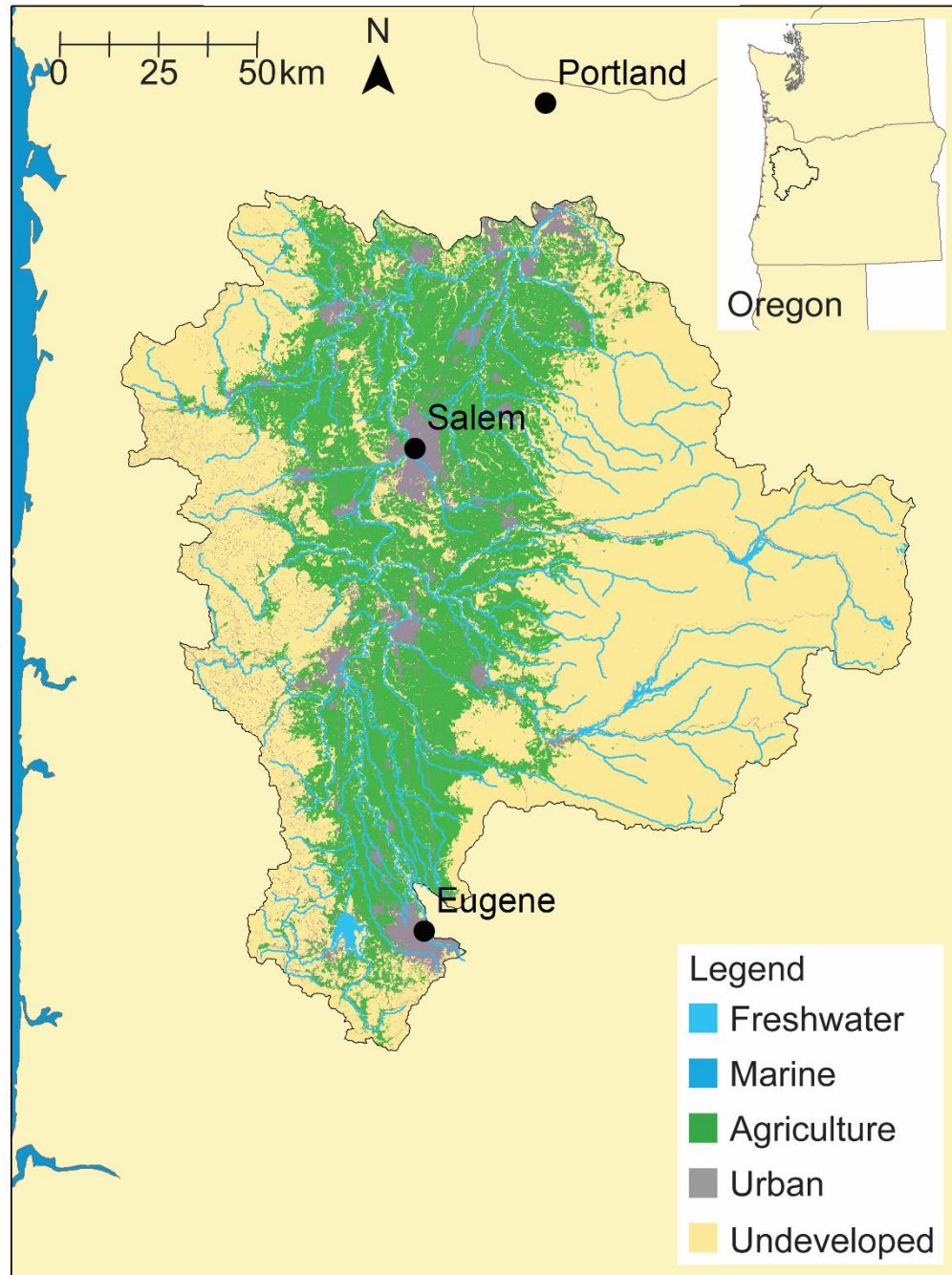
San Francisco, California



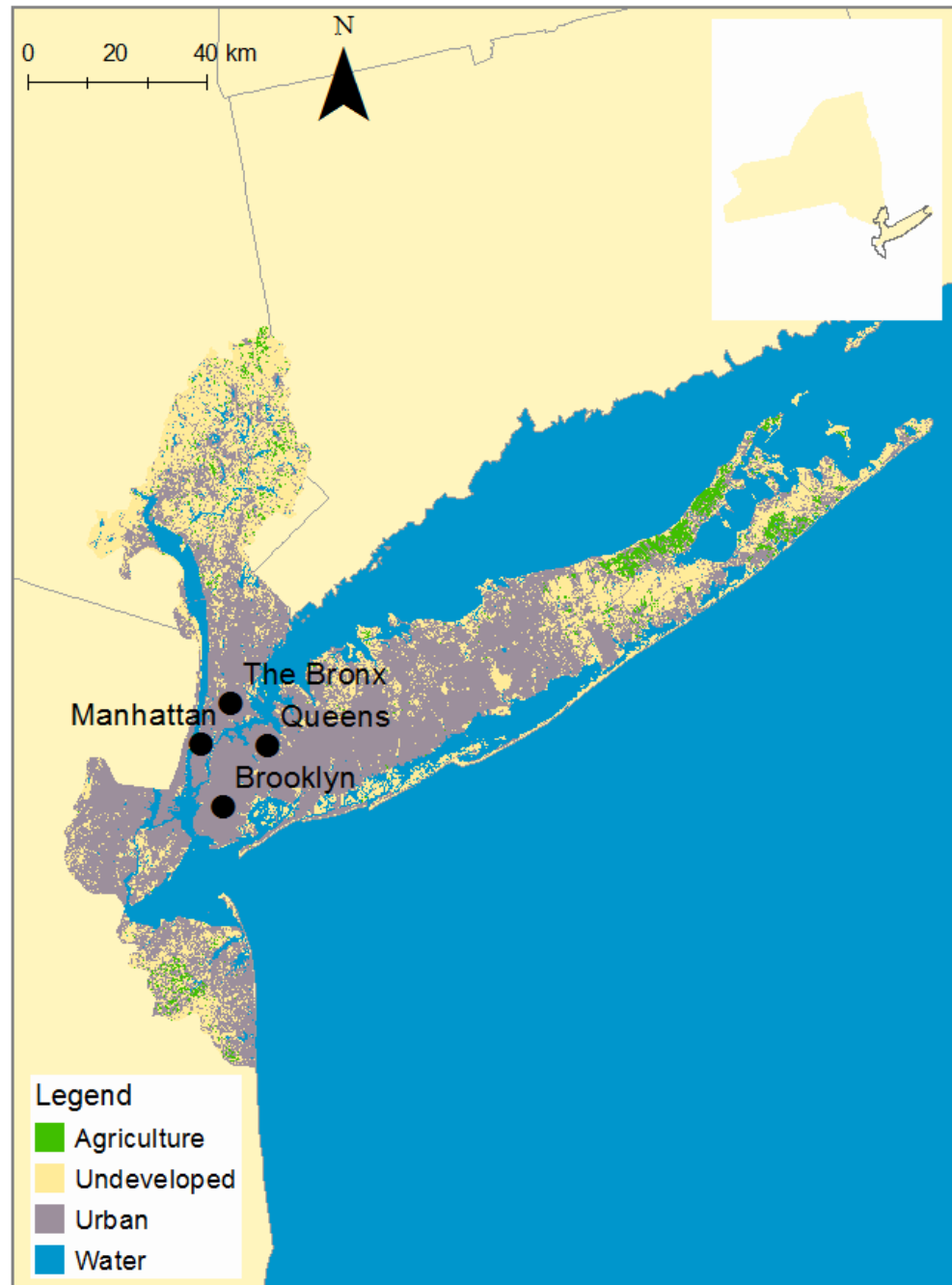
Visalia, California



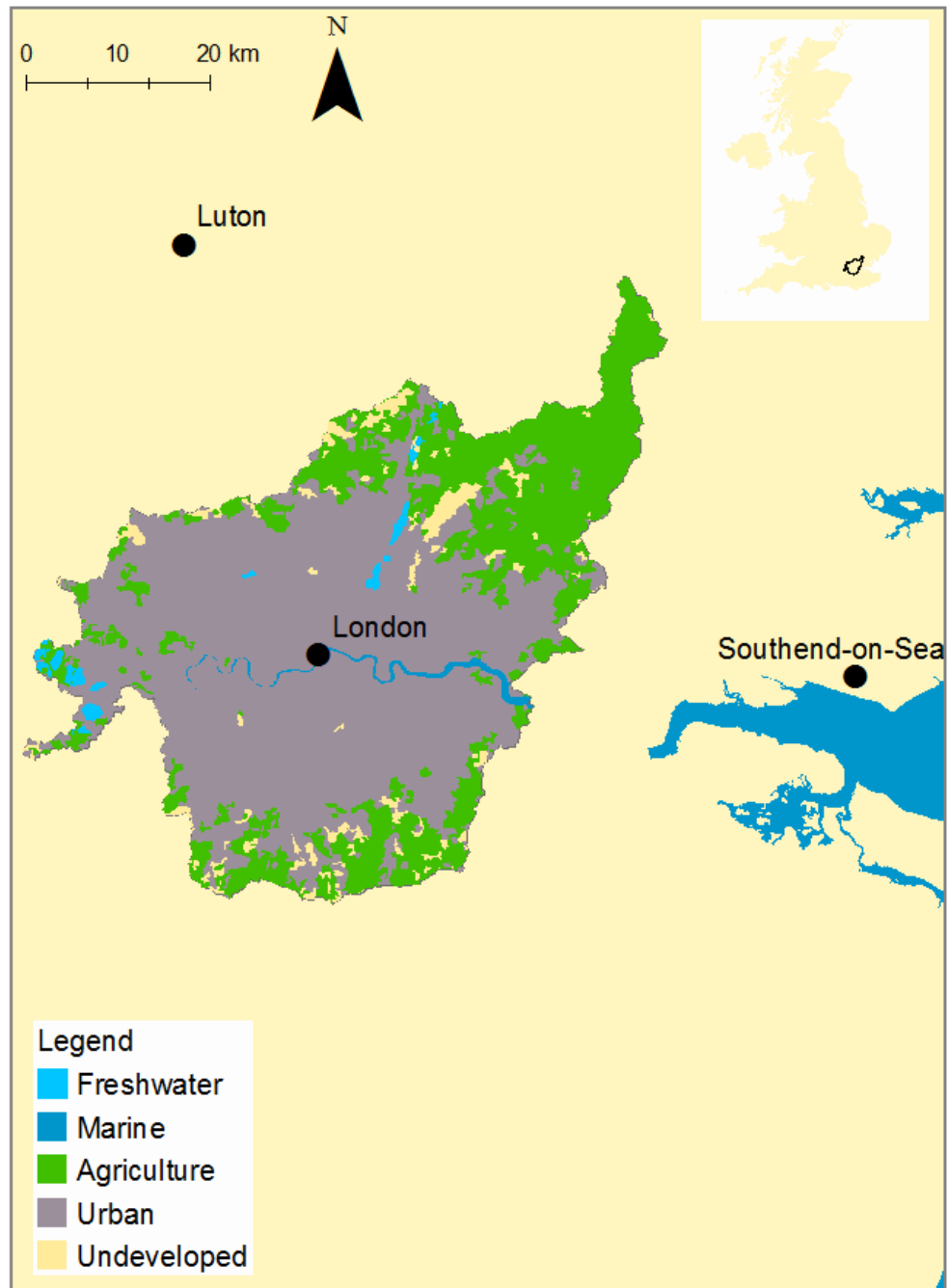
Salem, Oregon



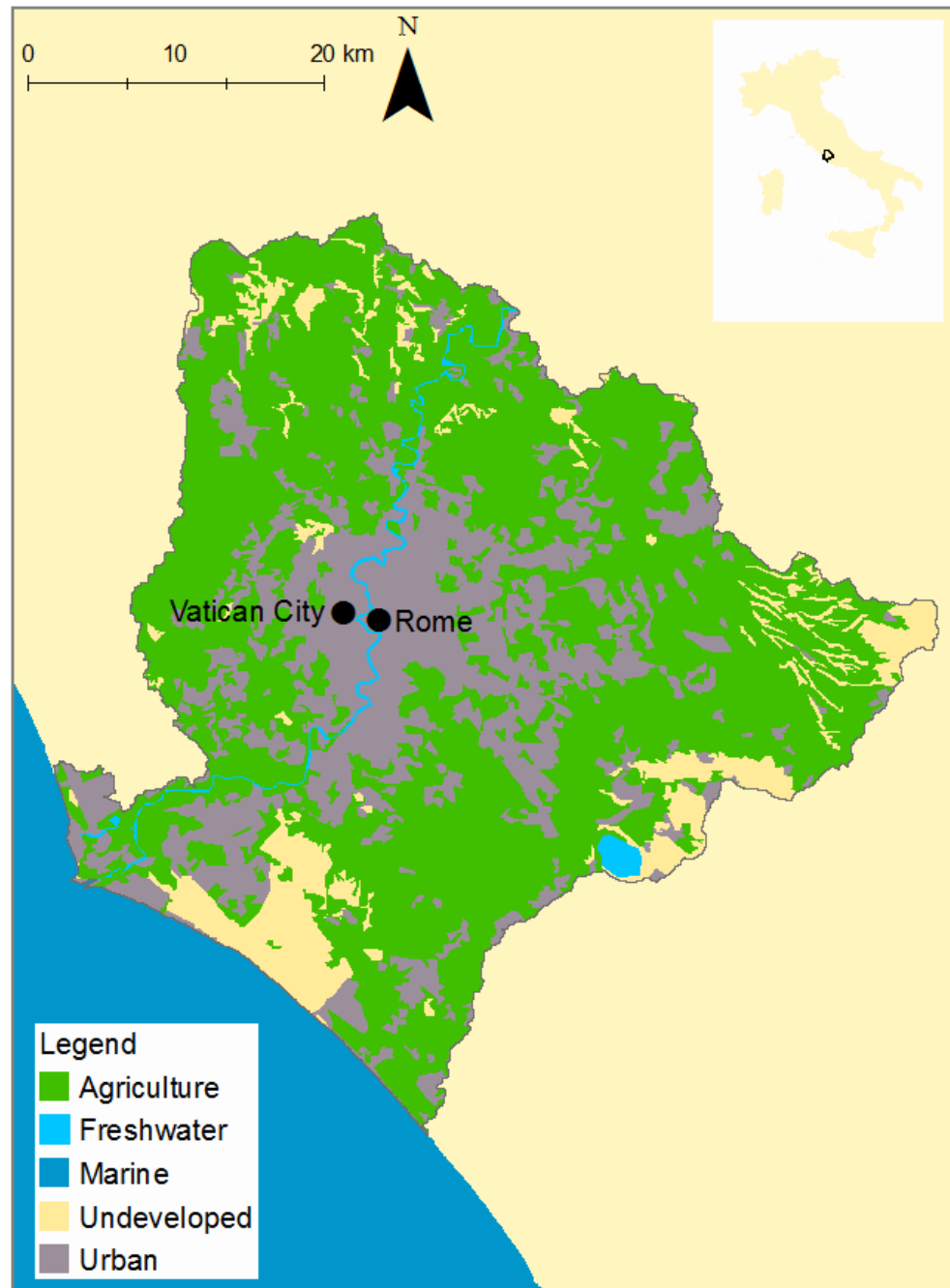
New York City, New York



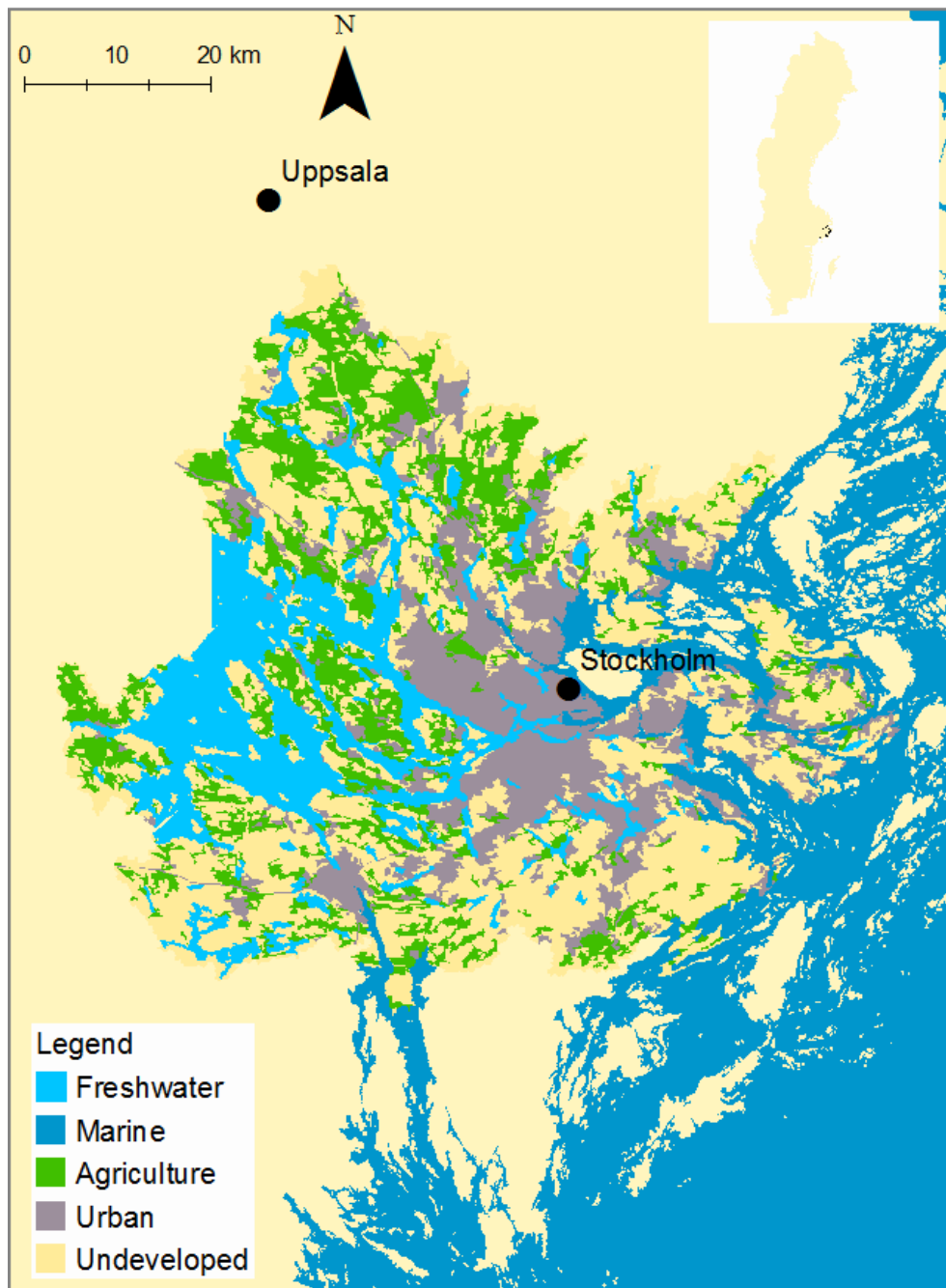
London, United Kingdom



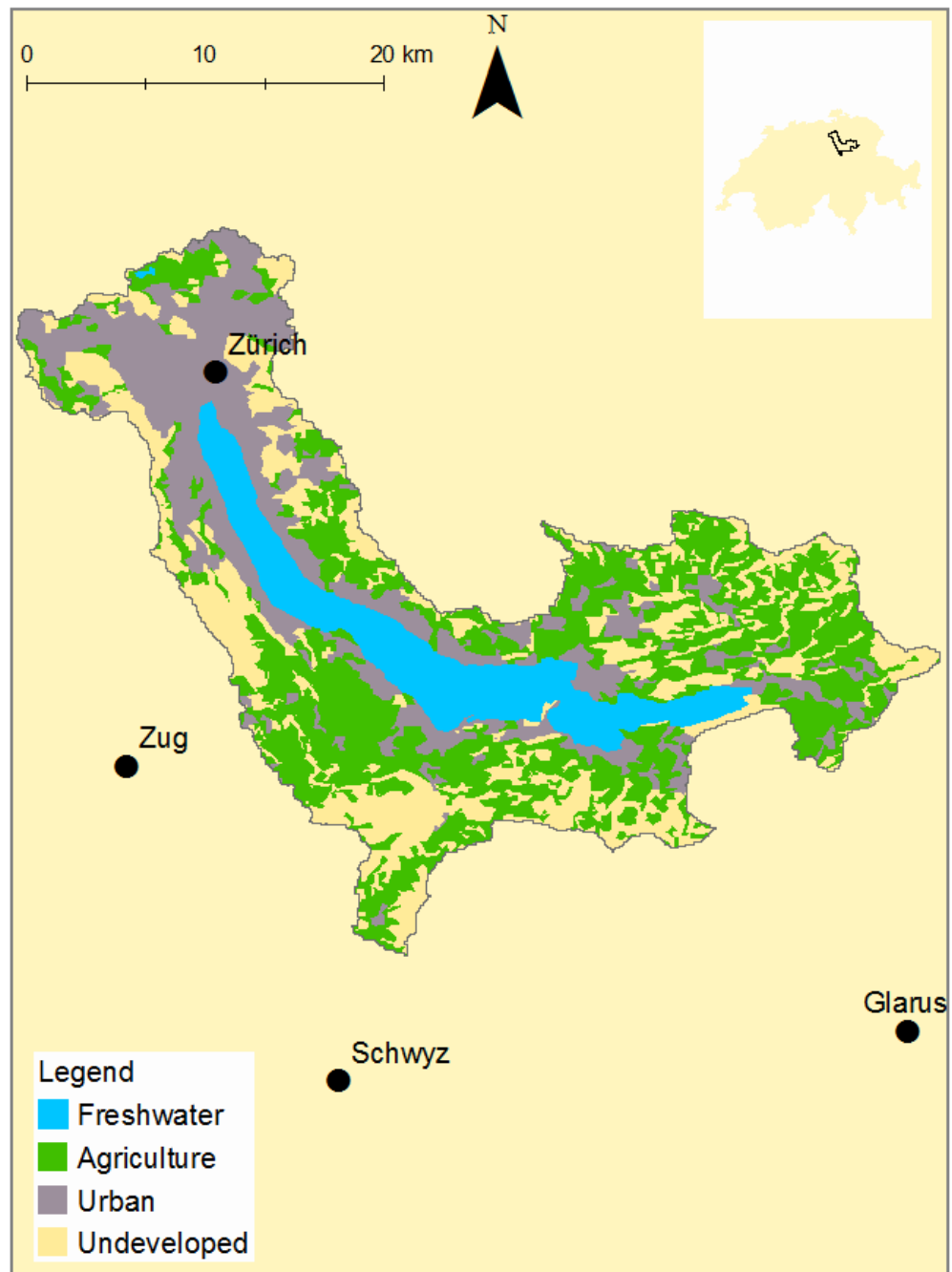
Rome, Italy



Stockholm, Sweden



Zurich, Switzerland



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