AA GeoEnvironmental Technical White Paper
PFAS Atmospheric Deposition and Transport Modeling

Atmospheric Models, Cross-Media Fate, Governing Equations, Calibration, Sensitivity, Validation, Uncertainty, Assumptions, and Limitations

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Purpose. This white paper presents a detailed technical framework for modeling PFAS emissions to air, atmospheric transport and deposition, and subsequent cross-media transfer to soil, surface water, and groundwater. It is designed for independent technical review, conceptual model development, remedial planning, and risk evaluation.

Prepared for professional technical review and decision support.

Executive Summary

PFAS atmospheric modeling integrates emission characterization, atmospheric physics, chemistry, and multimedia fate. A technically sound analysis must distinguish between volatile or semi-volatile neutral PFAS and low-volatility ionic PFAS, must account for gas-particle partitioning and deposition, and must evaluate whether atmospheric loading is an important contributor to soil, surface-water, food-chain, or groundwater exposure.

No universal air model is optimal for all PFAS issues. AERMOD is typically suited for near-field steady-state regulatory and screening applications. CALPUFF and SCICHEM are more appropriate for scenarios involving non-steady winds, complex terrain, shoreline effects, and the dynamics of evolving puffs. CMAQ and CAMx are regional three-dimensional chemistry-transport models designed for extensive domains, long-range transport, and comprehensive deposition analysis. The appropriate model selection is contingent upon scale, physics, chemistry, data, and the prediction to be substantiated.

This white paper presents the core mathematical equations behind PFAS air transport and deposition, practical interpretation of each equation, a cross-media framework linking air to soil and water, and a defensibility workflow covering calibration, validation, sensitivity analysis, uncertainty analysis, assumptions, and limitations.

Bottom line. A compelling PFAS atmospheric model is not the one with the most software features. It is the one whose governing equations, input data, parameterization, and uncertainty treatment are appropriate to the site, scale, and decision.

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1. Purpose, Scope, and Conceptual Model Foundations

Modeling of PFAS atmospheric deposition addresses questions such as: Do stack or fugitive air emissions result in quantifiable soil loading downwind? What proportion of environmental PFAS in soil or surface water can be attributed to atmospheric deposition compared to direct source release or biosolid applications that ultimately lead to groundwater contamination? Is the near-field industrial plume the primary contributor, or does regional background play a more significant role? Do atmospheric releases significantly alter human exposure through inhalation or drinking water? Defensible answers to those questions require a clearly defined conceptual site model.

A robust conceptual model identifies emission sources, emitted chemical classes, the nature of emissions (gaseous, particulate, or mixed), meteorological influences, deposition pathways, receiving media, and the relevant decision-making scale. The conceptual model for PFAS must differentiate between neutral volatile or semi-volatile precursors, such as fluorotelomer alcohols and sulfonamides, and ionic PFAS, which predominantly associate with particles or droplets and exhibit distinct deposition patterns.

The atmospheric pathway should also be viewed as one component of a multimedia PFAS system. Atmospheric releases can deposit directly to soil or water, accumulate in surficial soil, be remobilized by runoff or erosion, leach through the vadose zone, or contribute to background conditions over broad areas. Research notes that atmospheric transport and deposition occur on regional and global scales.

Professional interpretation. The most frequent mistake in PFAS air modeling is starting with a model before determining if atmospheric deposition is likely to be the primary pathway compared to direct wastewater discharge, landfill leachate, biosolids application, or groundwater transport.

2. PFAS Atmospheric Sources, Phases, and Cross-Media Pathways

Atmospheric PFAS sources include manufacturing stacks, thermal treatment units, fluoropolymer processing, coating operations, waste handling, wastewater treatment, landfills, sea-spray aerosol, and secondary formation from transformation of neutral precursors. Recent reviews emphasize that both primary sources and secondary sources matter, and that volatility and gas-particle partitioning are central to how PFAS move in the atmosphere.

Once emitted, PFAS may be present in the gas phase, associated with aerosol particles, or partitioned between the two. Gas-phase transport often dominates for more volatile neutral PFAS and can support longer-range movement. Particle-associated transport can matter for ionic PFAS and low-volatility compounds, especially where sources produce droplets, condensable material, or contaminated particulates. Deposition occurs by dry settling, surface uptake, and wet scavenging by cloud or rain processes.

The atmospheric processes are directly linked to cross-media transport. Deposition to soil can establish a surface reservoir, while deposition on impervious surfaces may be directed to stormwater systems. Additionally, deposition in lakes and rivers can lead to surface-water exposure, and deposition in recharge zones can gradually enhance groundwater loading. PFAS atmospheric modeling is most effective when incorporated into a multimedia mass-balance framework rather than considered as a standalone air assessment.

Cross-media perspective. Atmospheric deposition should be evaluated as a loading term to environmental media, not just as an air concentration outcome. The defensible prediction is often mass loading per area and time, not only an ambient air concentration contour.

3. Governing Equations - Atmospheric Deposition and Transport

Generally, atmospheric models solve or approximate conservation of mass for pollutant concentration in moving air, coupled with deposition, chemical transformation, emissions, and in some cases phase partitioning. The generic three-dimensional advection-diffusion-reaction equation presented in this white paper is the conservation backbone for advanced atmospheric PFAS models.

This equation may be solved directly in Eulerian models such as CMAQ or CAMx, or approximated analytically or semi-analytically in Gaussian plume and puff models. For PFAS, the governing form remains the same, but the way the source term, loss term, and deposition parameters are represented depends strongly on chemical class and available data.

If the atmosphere is represented as a steady-state plume from a continuous source, time dependence is dropped and turbulence is represented through stability-dependent dispersion parameters. If the release is represented as puffs moving through a time-varying wind field, the solution follows each puff in a Lagrangian frame. If the objective is regional chemical transport, the full three-dimensional conservation law is retained on a grid.

4. AERMOD Gaussian-Plume Modeling

The American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD) is a near-field dispersion model. It is a steady-state plume model with modern boundary-layer treatment provided by AERMET and terrain handling provided by AERMAP. In PFAS work, AERMOD is often used for near-field stack or fugitive releases where the domain is local, and the objective is ambient concentration or deposition screening under relatively stationary meteorology over each hour.

The underlying analytical idea is the Gaussian plume, shown below in its classical form. Modern AERMOD is more sophisticated than this compact equation: it includes boundary-layer scaling, plume rise, terrain interaction, building downwash, deposition options, and multiple source types. Still, the Gaussian-plume form remains the conceptual anchor for understanding how the model behaves.

For PFAS, AERMOD is usually applied as a physically simplified near-field model. Emissions may be treated as gas, particle, or a split between the two. Deposition may be represented conservatively using gas-phase assumptions, particle deposition, or both, depending on the chemical form and source process. Because PFAS chemistry in air is still an evolving field, a defensible AERMOD analysis usually focuses on near-field transport and deposition rather than detailed multiphase reaction chemistry.

AERMOD. AERMOD is most suitable for local or near-field industrial releases, compliance-style screening, and relatively stationary hourly winds. It is weaker for recirculating flow, long-range transport, or cases where PFAS chemistry and phase change drive the result.

5. CALPUFF and Gaussian-Puff Modeling

CALPUFF is a non-steady-state Lagrangian puff model. Instead of assuming one stationary plume for each hour, it releases advective puffs through a time- and space-varying meteorological field. This makes it useful for long-range transport, coastal effects, stagnation, recirculation, and situations where the wind field changes materially over the travel time of the pollutant.

A generic Gaussian-puff representation for a single puff is shown below. The puff center is advected in time by the wind field, and additional terms represent deposition, chemistry, and gravitational settling. CALPUFF is often used where plume travel time is long enough that meteorology cannot reasonably be treated as steady over the path.

For PFAS, CALPUFF can be attractive when emissions are local-to-regional, terrain or shoreline effects are important, and deposition to land or water is a key output. Because puff models can use gridded land-use and meteorological fields, they often provide more realistic deposition footprints than a simple steady plume where complex winds dominate.

PFAS relevance. CALPUFF is often a good bridge between local plume models and full regional chemistry-transport models when the main question is downwind deposition rather than detailed atmospheric chemical transformation.

6. CMAQ and CAMx Eulerian Chemistry-Transport Modeling

The Community Multiscale Air Quality (CMAQ) and Comprehensive Air quality Model with extensions (CAMx) are three-dimensional Eulerian grid models that solve the advection-diffusion-reaction equation on a regional domain. They are designed for multi-day to multi-year simulations, gridded emissions, cloud and precipitation processes, dry and wet deposition, and atmospheric chemistry. These models are the appropriate tools when the problem extends beyond a local plume footprint, and the question involves long-range transport, regional background, cumulative deposition, or chemistry-driven transformation.

CMAQ has recently been extended by EPA researchers to simulate a broad PFAS suite from a fluoropolymer manufacturing source, specifically to investigate regional-scale deposition and ambient air exposure. EPA notes that most earlier PFAS air modeling had focused on plume models over only tens of kilometers, and that CMAQ makes it possible to examine larger spatial scales and more chemically resolved PFAS suites. CMAQ-PFAS model is used for modeling regional background PFAS loading, PFAS emissions from fluoropolymer manufacturing facilities, atmospheric transport of fluorotelomer alcohols, formation of perfluorocarboxylic acids, PFAS deposition to surface water, as well as watershed-scale deposition.

CAMx is conceptually similar as a regional Eulerian model and includes source apportionment and direct sensitivity tools that are valuable for deposition studies. Its decoupled direct method can compute first-order sensitivities to emissions and parameters without requiring many separate brute-force runs. For PFAS, Eulerian regional models are particularly useful when the objective is annual or seasonal deposition to watersheds, long-range background contribution, comparison of candidate emission inventories, or evaluation of source contributions over broad domains.

Regional-scale takeaway. CMAQ and CAMx are not just bigger dispersion models. They are conservation-of-mass chemistry-transport frameworks appropriate when PFAS deposition must be evaluated as a regional or cumulative burden.

7. SCICHEM and Other Advanced Puff Approaches

SCICHEM is a Lagrangian reactive puff model often used where chemical transformation, terrain, and non-steady winds matter but the analyst does not need a full continental-scale Eulerian model. In PFAS applications, SCICHEM can be useful for local to regional domains with time-varying meteorology, coastal effects, or more refined treatment of puff chemistry and deposition than a simple Gaussian plume.

The conceptual governing equation is still a moving-puff mass balance with advection, turbulent spread, deposition, and reaction. In practical PFAS work, SCICHEM is most attractive where users want a Lagrangian model with richer process options than a steady-state plume but without the full complexity of a regional chemical transport model (CTM).

More broadly, model selection should follow physics and scale: puff models for evolving local-to-regional plumes and complex winds, Eulerian CTMs for cumulative regional burden, and steady Gaussian plume models for near-field screening or regulatory-style applications.

8. Cross-Media - Transfer to Soil, Surface Water, and Groundwater

Atmospheric PFAS modeling becomes most useful when converted to multimedia loading and fate. The deposition flux predicted by an air model can be treated as an aerial source to soil, surface water, or a watershed mass-balance model. That step is what links air releases to actual environmental concentrations and receptor exposure.

A simple soil-surface mass balance, a surface-water mass balance, and a recharge-linked groundwater loading term are provided below. These equations are intentionally lumped. They are not substitutes for a vadose-zone or groundwater flow-and-transport model, but they provide a defensible bridge between air-model outputs and down-gradient environmental consequences.

In many site assessments, this cross-media step is the most important analytical bridge in the entire chain. If deposition to soil is small relative to direct wastewater discharge or biosolids loading, the air pathway may be secondary. If deposition is persistent and widespread, however, it can become the controlling source term for diffuse environmental burdens.

Cross-media red flag. A common weakness is to stop at atmospheric concentration contours and never convert deposition to a receiving-media load. That often leaves the key environmental question unanswered.

9. Calibration and Inverse Modeling with PEST and Related Tools

Atmospheric PFAS models are commonly calibrated or constrained using ambient air concentrations, deposition measurements, rain chemistry, stack test data, meteorological observations, and, in some cases, downwind soil concentrations or multimedia mass-balance evidence. Inverse modeling can be used to estimate emissions, phase splits, deposition velocities, scavenging coefficients, or other uncertain parameters by matching model outputs to observations.

PEST can be wrapped around atmospheric models in the same way it is wrapped around groundwater models: a run script generates the model input, runs the executable, extracts objective outputs, and compares them to targets. In PFAS air modeling, the parameters most plausibly estimated this way are emissions by species group, gas-particle split fractions, deposition velocities, effective scavenging coefficients, source release heights, or uncertain temporal emissions profiles.

The analyst should be cautious, however, because atmospheric inverse problems can be strongly nonunique. Different emissions and deposition parameter combinations may produce similar air concentrations but very different deposition footprints. For that reason, calibration targets should include deposition data whenever deposition is the prediction of interest.

Calibration principle. A PFAS atmospheric model should be calibrated to the variable that matters for the decision. If the decision is about soil loading, calibrating only to air concentrations may be insufficient.

10. Sensitivity Analysis and Validation

Sensitivity analysis identifies which parameters most control predictions such as annual deposition, maximum monthly deposition, ambient concentration, or multimedia loading. Local and global methods are both useful. Local derivatives help determine which parameters matter near the calibrated solution. Morris and Sobol methods help reveal nonlinearity, parameter interactions, and global importance across realistic prior ranges.

In PFAS atmospheric applications, high-sensitivity parameters commonly include emissions magnitude, temporal emissions profile, gas-particle partitioning assumptions, deposition velocity, scavenging coefficient, particle size distribution, and uncertainty in the chemical specificity of the emission inventory. EPA researchers reported that decreasing the chemical specificity of PFAS emissions had the largest effect on modeled deposition in their regional CMAQ study.

Validation should be multi-metric and multi-variable. A model can match average air concentrations and still miss deposition. Corroboration should therefore use ambient air, rainwater concentrations, dry deposition if measured, and where possible the spatial gradient in surficial soil or water-body burden.

Validation reality check. A good-looking contour plot is not validation. Validation requires comparison against independent observations relevant to the model's intended use, ideally including both air concentration and deposition data.

11. Uncertainty Analysis and Predictive Defensibility

Parameter covariance, first-order variance propagation, Monte Carlo propagation, and posterior-style updating all have a role in PFAS atmospheric modeling. For most practical applications, uncertainty in emissions is at least as important as uncertainty in the transport code. Sensitivity and uncertainty analysis should therefore explicitly examine alternative emissions inventories, source speciation, and gas-particle phase assumptions.

Structural uncertainty must also be acknowledged. A steady-state plume model may be structurally inadequate where shoreline recirculation matters. A regional Eulerian CTM may be structurally unnecessary where the decision is only a near-field screening question. For PFAS, structural uncertainty also arises from incomplete knowledge of atmospheric transformation pathways and imperfect phase-partitioning data.

The defensible final product is therefore not a single contour map. It is a prediction range conditioned on realistic alternatives in emissions, phase split, deposition parameterization, and model class.

Defensibility principle. A single deterministic PFAS deposition map should almost never be the final answer. The defensible answer is a range conditioned on realistic alternative emissions and process assumptions.

12. Assumptions, Limitations, and Conclusions

Key assumptions and limitations should be disclosed in the main body of the report rather than hidden in an appendix. Analysts should clearly state how PFAS are represented chemically, whether deposition is gas-phase, particle-phase, or mixed, how precipitation scavenging is treated, what data support the emissions inventory, and whether atmospheric deposition is likely to dominate or merely supplement other source pathways.

Common limitations include sparse deposition data, uncertain emissions profiles, incomplete PFAS speciation, and nonunique cross-media interpretations. Common errors include using a near-field plume model to make long-range claims, treating all PFAS as one generic compound without sensitivity analysis, calibrating only to air concentrations when deposition is the key prediction, and reporting one deterministic forecast with no uncertainty treatment.

The central conclusion of this white paper is that PFAS atmospheric modeling is most defensible when it is treated as a mass-loading and multimedia transport problem, not merely an air-concentration mapping exercise. The right model class depends on scale and process; the right calibration targets depend on the decision; and the right communication style is explicit about uncertainty.

Core Mathematical Equations

Equation 3-1. General atmospheric advection-diffusion-reaction-deposition equation.

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}\, C) = \nabla \cdot (\mathbf{K}\, \nabla C) + S - L - \Lambda_w C - \nabla \cdot (\mathbf{v}_s\, C)$$

Where:

C = air concentration [M/L^3]

t = time [T]

u = wind velocity vector [L/T]

K = eddy diffusivity tensor [L^2/T]

S = emission source term [M/L^3/T]

L = chemical or other loss term [M/L^3/T]

Λ_w = first-order wet-scavenging coefficient [1/T]

$\mathbf{v}_s$ = settling velocity vector, commonly vertical [L/T]

Equation 3-2. Gas-particle partition coefficient.

$$K_p = \frac{C_p}{\mathrm{TSP}\, C_g}$$

Where:

K_p = particle/gas partition coefficient

C_p = particle-phase concentration

C_g = gas-phase concentration

TSP = total suspended particulates

Equation 3-3. Henry-law style air-water partition relationship.

$$H = \frac{C_{\text{air}}}{C_{\text{water}}}$$

Where:

H = Henry coefficient in the formulation used

C_{air} = concentration in air

C_{water} = concentration in water

Equation 3-4. Dry deposition flux.

$$F_d = V_d\, C_a$$

Where:

F_d = dry deposition flux [M/L^2/T]

V_d = deposition velocity [L/T]

C_a = air concentration at reference height [M/L^3]

Equation 3-5. First-order wet scavenging.

$$\frac{dC}{dt} = -\Lambda C$$

Where:

Λ = bulk scavenging coefficient [1/T]

Equation 3-6. Wet deposition flux.

$$F_w = P\, C_r$$

Where:

F_w = wet deposition flux [M/L^2/T]

P = precipitation rate [L/T]

C_r = concentration in rainwater [M/L^3 water]

Equation 3-7. Total deposition flux.

$$J_{\text{dep}} = F_d + F_w$$

Where:

J_{dep} = total atmospheric deposition flux [M/L^2/T]

AERMOD / Near-Filed Dispersion Modeling

Facility-scale dispersion is often modeled using Gaussian plume equations.

Equation 4-1. Classical Gaussian-plume concentration.

$$C(x,y,z) = \frac{Q}{2\pi U\,\sigma_y \sigma_z}\,\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right]$$

Where:

Q = emission rate [M/T]

U = mean wind speed at stack height [L/T]

σ_y, σ_z = lateral and vertical dispersion parameters [L]

H = effective stack height including plume rise [L]

Equation 4-2. Effective stack height.

$$H = h_s + \Delta h$$

Where:

h_s = physical stack height [L]

Δh = plume rise [L]

CALPUFF / Time-Dependent Regional Transport

Gaussian-puff, non-steady steady state, Lagrangian model. It represents emissions as moving puffs.

Equation 5-1. Gaussian-puff concentration for a moving puff.

$$C(x,y,z,t) = \frac{M_p}{(2\pi)^{3/2}\,\sigma_x\sigma_y\sigma_z} \exp\left(-\frac{\left(x-x_p\right)^2}{2\sigma_x^2}\right)\exp\left(-\frac{\left(y-y_p\right)^2}{2\sigma_y^2}\right)\exp\left(-\frac{\left(z-z_p\right)^2}{2\sigma_z^2}\right)$$

Where:

$\mathbf{M_p}$ = mass in the puff [M]

$\mathbf{x_p, y_p, z_p}$ = puff-center coordinates [L]

$\boldsymbol{\sigma_x, \sigma_y, \sigma_z}$ = puff spread parameters [L]

Equation 5-2. Puff-center advection and settling.

$$\frac{dx_p}{dt} = u_x, \qquad \frac{dy_p}{dt} = u_y, \qquad \frac{dz_p}{dt} = u_z - v_s$$

Where:

$\mathbf{u_x, u_y, u_z}$ = wind-speed components [L/T]

$\mathbf{v_s}$ = settling velocity [L/T]

This model captures changing wind direction, meteorological variability, complex terrain, and regional transport.

SCICHEM — Reactive Puff Modeling

This model represents major advancement over gaussian model.

$$\frac{\partial C}{\partial t} + \mathbf{U} \cdot \nabla C = \nabla \cdot (K\nabla C) + R(C)$$

Where:

- K = turbulent diffusivity tensor
- $R(C)$ = chemical reaction term

It includes chemical transformation, gas-particle partitioning, multi-phase behavior, different emission mixtures, complex terrain, and urban canopy effects. SCICHEM model particularly relevant when PFAS precursors (e.g., FTOHs) undergo atmospheric oxidation prior to deposition.

CMAQ / CAMx (Eulerian chemistry-transport equations)

Equation 6-1. Eulerian chemistry-transport equation.

$$\frac{\partial C_i}{\partial t} = -\nabla \cdot (\mathbf{u}C_i) + \nabla \cdot (K\nabla C_i) + E_i + P_i - L_i - D_i$$

$$\frac{\partial C_i}{\partial t} = -\left(\frac{\partial (uC_i)}{\partial x} + \frac{\partial (vC_i)}{\partial y} + \frac{\partial (wC_i)}{\partial z}\right) + \frac{\partial}{\partial x}\left(K_x \frac{\partial C_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial C_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial C_i}{\partial z}\right) + E_i + P_i - L_i - D_i$$

Where:

- Ci = grid-cell concentration of species i
- u = wind vector
- K = eddy diffusivity tensor
- Ei = emissions term
- P_i = Chemical production
- Li = chemical loss term
- Di = dry and wet deposition or other removal

Equation 6-2. Direct first-order sensitivity equation.

$$\frac{\partial S_j}{\partial t} = -\nabla \cdot \left(\mathbf{u}\, S_j\right) + \nabla \cdot \left(\mathbf{K}\, \nabla S_j\right) + \frac{\partial E}{\partial p_j} + \left(\frac{\partial R}{\partial C}\right) S_j + \frac{\partial R}{\partial p_j} - \frac{\partial D}{\partial p_j}$$

Where:

S_j = first-order sensitivity of concentration to parameter pj, that is ∂C/∂pj

CAMx combines chemistry into a single $R_i$term, unlike CMAQ that separates chemical processes into $P_i - L_i$. This major difference is a result of numerical solver design, not their fundamental physical processes.

Cross-media equations

Equation 8-1. Deposition physics and soil boundary conditions

Atmospheric deposition flux:

$$J(x, y, t) = V_d C + \Lambda C$$

Integrated mass to soil:

$$M_{soil}(t) = \int_0^t J(x, y, \tau)d\tau$$

Vadose boundary conversion:

$$C_{surface}(t) = \frac{J}{\rho_b \theta}$$

Where

J = atmospheric deposition flux

ρ_b = soil bulk density

θ = soil volumetric moisture content

Equation 8-2. Vadose Zone Transport.

Advection–dispersion–sorption:

$$\frac{\partial C_s}{\partial t} = \nabla \cdot (D\nabla C_s) - v\frac{\partial C_s}{\partial z} - \mu C_s + \frac{J}{\rho_b}$$

PFAS linear (equilibrium) sorption:

$$\left(1+\frac{\rho_b K_d}{\theta}\right)\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C) - v\frac{\partial C}{\partial z} - \mu C + \frac{J}{\rho_b}$$

PFAS rate limited (non-equilibrium) sorption:

$$\theta\frac{\partial C}{\partial t} + \rho_b \alpha(K_d C - S_2) = \nabla \cdot (D\nabla C) - v\frac{\partial C}{\partial z} - \mu C + J$$

PFAS air-water interfacial adsorption:

$$\left(1+\frac{\rho_b K_d}{\theta}+\frac{K_{aw} A_{aw}}{\theta}\right)\frac{\partial C_s}{\partial t} = \nabla \cdot (D\nabla C_s) - v\frac{\partial C_s}{\partial z} - \mu C_s + \frac{J}{\rho_b}$$

For PFAS vadose-zone transport with **linear sorption, rate-limited sorption, and air-water interfacial adsorption**.

$$\left(1+\frac{\rho_b K_d}{\theta}+\frac{K_{aw}A_{aw}}{\theta}\right)\frac{\partial C}{\partial t}+\rho_b\alpha(K_d C-S_2)=\nabla\cdot(D\nabla C)-v\frac{\partial C}{\partial z}-\mu C+J$$

Where:

C_s = soil contaminant concentration (e.g., PFAS)

t = time evolution of soil contamination

D = effective soil diffusion/dispersion coefficient

v = vertical pore-water velocity

z = vertical coordinate

μ = first-order decay/transformation

K_d = distribution coefficient

K_{aw} = interfacial adsorption coefficient

A_{aw} = air-water interfacial area

Equation 8-3. Surficial-soil PFAS mass balance.

$$\frac{dM_s}{dt}=A\,J_{\text{dep}}+A\,J_{\text{irrig}}-k_{\text{leach}}M_s-k_{\text{runoff}}M_s-k_{\text{deg}}M_s-k_{\text{vol}}M_s$$

Where:

M_s = PFAS mass in the soil control volume [M]

A = receiving area [L^2]

J_{dep} = atmospheric deposition flux [M/L^2/T]

J_{irrig} = optional irrigation or other external loading flux

k_{leach} = effective first-order leaching loss rate [1/T]

k_{runoff} = effective first-order runoff/erosion loss rate [1/T]

k_{deg} = effective degradation or transformation rate [1/T]

k_{vol} = effective volatilization rate for volatile precursors [1/T]

Equation 8-4. Surface-water mass balance with atmospheric loading.

$$\frac{dM_w}{dt} = A_w J_{\text{dep}} + Q_{\text{run}} C_{\text{run}} + Q_{\text{gw}} C_{\text{gw}} - Q_{\text{out}} C_w - k_{\text{deg},w} M_w - k_{\text{sed}} M_w$$

Where:

M_w = PFAS mass in the water body [M]

A_w = water-surface area [L^2]

Q_{run} = runoff inflow [L^3/T]

C_{run} = PFAS concentration in runoff [M/L^3]

Q_{gw} = groundwater inflow [L^3/T]

C_{gw} = PFAS concentration in groundwater inflow [M/L^3]

Q_{out} = surface-water outflow [L^3/T]

C_w = water-column concentration [M/L^3]

$k_{deg,w}$ = effective degradation/transformation rate in water [1/T]

k_{sed} = effective settling or sedimentation rate [1/T]

Equation 8-3. Recharge mass flux to groundwater.

$$J_{\text{gw}} = q_r \, C_{\text{pore}}$$

Where:

J_{gw} = PFAS mass flux to groundwater [M/L^2/T]

q_r = recharge rate [L/T]

C_{pore} = PFAS concentration in infiltrating pore water [M/L^3]

A simplified weighted-groundwater recharge boundary for conservative screening estimates is given in the below equation:

$$C_{recharge} = \frac{1}{R}\int J dt$$

This equation assumes that all deposited PFAS mass reaching soil is diluted only by groundwater recharge, which represents water flux transporting PFAS downward to the underlying aquifer. For more realistic screening, the equation becomes:

$$C_{\text{recharge}} = \frac{1}{R}\int \frac{J\, f_{\text{inf}}}{1 + \frac{\rho_b K_d}{\theta} + \frac{K_{aw} A_{aw}}{\theta}} e^{-\mu t}\, dt$$

For site-specific modeling beyond preliminary screening, particularly in the presence of macropores or fractures, the above equation can be modified as follows to include vadose-zone travel time t_v and preferential flow fraction f_{pf} (optional):

PFAS travel time through vadose zone:

$$t_v = \frac{L R_f}{v}$$

PFAS potential preferential flow:

$$f_{pf} = \frac{q_{pf}}{q}$$

Combined equation:

$$C_{recharge,pf} = \frac{1}{R}\int \frac{J f_{inf}(1 + f_{pf})}{1 + \frac{\rho_b K_d}{\theta} + \frac{K_{aw} A_{aw}}{\theta}} e^{-\mu(t - t_v)}\, dt$$

Where:

C_{recharge} = groundwater recharge concentration

f_{inf} = Infiltration fraction

R = groundwater recharge rate

R_f = retardation factor

t_v = travel time

$e^{-\mu t}$ = degradation or transformation

$e^{-\mu(t-t_v)}$ = attenuation during transport

L = vadose zone thickness

q_{pf} = preferential flow flux

q = total infiltration flux

Numerical Methods and Operator Splitting

Finite-difference numerical discretization typically used in chemical transport models (CTMs) such as CMAQ and CAMx to solve the atmospheric advection-diffusion-reaction equation.

Continuous Governing Equation

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} - w\frac{\partial C}{\partial z} + \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + S - D + R$$

Grid Representation

CTMs divides the atmosphere into 3-D grid cells (i, j, k)

representing

- longitude (x)
- latitude (y)
- vertical layer (z)

with spacing:

$$\Delta x,\ \Delta y,\ \Delta z$$

Time Discretization:

$$\frac{\partial C}{\partial t} \approx \frac{C_{i,j,k}^{n+1} - C_{i,j,k}^{n}}{\Delta t}$$

n current timestep

$n+1$ next timestep

Advection Discretization:

$$u\frac{\partial C}{\partial x} \approx u_{i,j,k}\frac{C_{i+1,j,k} - C_{i-1,j,k}}{2\Delta x}$$

Representing transport between neighboring grid cells.

Diffusion Discretization:

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) \approx K_x\frac{C_{i+1,j,k} - 2C_{i,j,k} + C_{i-1,j,k}}{\Delta x^2}$$

This term causes pollutant plume spreading.

Full Finite-Difference Equation:

$$\frac{C_{i,j,k}^{n+1} - C_{i,j,k}^{n}}{\Delta t} = -u\frac{C_{i+1,j,k} - C_{i-1,j,k}}{2\Delta x} - v\frac{C_{i,j+1,k} - C_{i,j-1,k}}{2\Delta y} - w\frac{C_{i,j,k+1} - C_{i,j,k-1}}{2\Delta z}$$

$$+K_x\frac{C_{i+1,j,k} - 2C_{i,j,k} + C_{i-1,j,k}}{\Delta x^2} + K_y\frac{C_{i,j+1,k} - 2C_{i,j,k} + C_{i,j-1,k}}{\Delta y^2} + K_z\frac{C_{i,j,k+1} - 2C_{i,j,k} + C_{i,j,k-1}}{\Delta z^2} + S - D + R$$

This presents the numerical solution obtained for each grid cell.

Operator Splitting Implementation

TMs rarely solve the complete equation at once. Instead, operator splitting technique is utilized.

$$C^{n+1} = D_{\Delta t} \circ C_{\Delta t} \circ T_{\Delta t}(C^n)$$

Transport step
↓
Chemistry step
↓
Deposition step

Each process updates the concentration sequentially. This illustrates computational transparency, which is a key aspect of defensible chemical transport modeling.

Calibration and Inverse-Model Equations

Equation 9-1. Weighted least-squares objective function.

$$\Phi(\mathbf{p}) = \sum_i w_i \left[y_i^{\text{obs}} - y_i(\mathbf{p})\right]^2$$

Where:

p = parameter vector

$\mathbf{y_i^{obs}}$ = observed value for target i

$\mathbf{y_i(p)}$ = modeled value for target i

$\mathbf{w_i}$ = observation weight, often 1/σ_i^2

Equation 9-2. Common weighting formula.

$$w_i = \frac{1}{\sigma_i^2}$$

Where:

$\boldsymbol{\sigma_i^2}$ = observation error variance

Equation 9-3. Regularized objective function.

$$\Phi_{\text{total}} = \Phi_{\text{obs}} + \mu\,\Phi_{\text{reg}}$$

Where:

μ = regularization weight

$\boldsymbol{\Phi_{reg}}$ = penalty term for deviation from preferred values or smoothness constraints

Equation 9-4. Parameter-update equation used in many inverse methods.

$$(\mathbf{J}^T\mathbf{WJ} + \lambda\mathbf{I})\Delta\mathbf{p} = \mathbf{J}^T\mathbf{Wr}$$

Where:

J = Jacobian or sensitivity matrix

W = weighting matrix

λ = damping factor

$\boldsymbol{\Delta_p}$ = parameter update vector

r = residual vector

Sensitivity and validation equations

Equation 10-1. Local sensitivity coefficient.

$$S_j = \frac{\partial Y}{\partial p_j}$$

Where:

Y = model output of interest

p_j = parameter j

Equation 10-2. Normalized local sensitivity coefficient.

$$S_j^* = \left(\frac{p_j}{Y}\right)\left(\frac{\partial Y}{\partial p_j}\right)$$

Where:

S_j* = dimensionless sensitivity measure

Equation 10-3. Finite-difference local sensitivity.

$$\frac{\partial Y}{\partial p_j} \approx \frac{Y(p_j + \Delta p_j) - Y(p_j - \Delta p_j)}{2\Delta p_j}$$

Where:

Δp_j = small perturbation in parameter p_j

Equation 10-4. Morris elementary effect.

$$EE_i(\mathbf{X}) = \frac{Y(X_1, \dots, X_i + \Delta, \dots, X_k) - Y(\mathbf{X})}{\Delta}$$

Where:

EE_i = elementary effect for factor i

Δ = step size in the normalized factor space

Equation 10-5. Morris summary statistics.

$$\mu_i^* = \frac{1}{r}\sum_j \left|EE_{i,j}\right|, \qquad \sigma_i = \sqrt{\frac{1}{r-1}\sum_j \left(EE_{i,j} - \mu_i\right)^2}$$

Where:

μ_i* = mean absolute elementary effect, indicating overall influence

σ_i = spread of effects, indicating nonlinearity or interactions

Equation 10-6. First-order and total-effect Sobol indices.

$$S_i = \frac{V_i}{\mathrm{Var}(Y)}, \qquad S_{T_i} = 1 - \frac{\mathrm{Var}_{X_{\sim i}}\left(E_{X_i}[Y \mid X_{\sim i}]\right)}{\mathrm{Var}(Y)}$$

Where:

V_i = variance contribution of parameter i

S_i = first-order sensitivity index

ST_i = total-effect sensitivity index

Equation 10-7. Mean bias.

$$MB = \frac{1}{n}\sum_i (P_i - O_i)$$

Where:

P_i = predicted value

O_i = observed value

Equation 10-8. Normalized mean bias.

$$NMB = 100\,\frac{\sum_i (P_i - O_i)}{\sum_i O_i}$$

Where:

NMB = percent normalized mean bias

Equation 10-9. Root mean square error.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i}(P_i - O_i)^2}$$

Where:

RMSE = root mean square error

Equation 10-10. Factor-of-two agreement metric.

$$FAC2 = \text{fraction of predictions satisfying } 0.5 \le \frac{P_i}{O_i} \le 2$$

Where:

FAC2 = fraction of model predictions within a factor of two of the observations

Equation 10-11. Willmott index of agreement.

$$IOA = 1 - \frac{\sum_i (P_i - O_i)^2}{\sum_i (|P_i - \bar{O}| + |O_i - \bar{O}|)^2}$$

Where:

IOA = index of agreement

$\bar{O}$ = mean observed value

Uncertainty Propagation Across Media

Equation 11-1. Probabilistic Structure.

Uncertain parameter vector

$$Y(x,t) = C_{gw}(x,t)$$

$$\theta = [Q, u, K, v_d, P, K_d, K_{aw}, A_{aw}, \theta, \rho_b, f_{inf}, R, L, v, D, \mu, \alpha, f_{pf}, \dots]$$

Entire cross-media system is:

$$Y = \mathcal{M}(\theta)$$

where $\mathcal{M}$ is the coupled model

Uncertainty-analysis equations

Equation 11-2. Linearized parameter covariance matrix.

$$\mathbf{C}_p = s^2(\mathbf{J}^T\mathbf{W}\mathbf{J})^{-1}$$

Where:

$\mathbf{C}_\mathbf{p}$ = parameter covariance matrix

s^2 = residual variance estimate

Equation 11-3. Residual variance estimator.

$$s^2 = \frac{\Phi(\mathbf{p}^*)}{n-m}$$

Where:

p* = optimal parameter set

n = number of observations

m = number of estimated parameters

Equation 11-4. First-order variance propagation for a prediction.

$$\mathrm{Var}(Z) \approx \mathbf{g}_p^T\,\mathbf{C}_p\,\mathbf{g}_p$$

Where:

$\mathbf{g}_\mathbf{p}$ = gradient vector of prediction Z with respect to the parameters

Equation 11-5. Monte Carlo uncertainty framework.

$$\mathbf{p}^{(k)} \sim f_p(\mathbf{p}), \qquad Y^{(k)} = f\left(\mathbf{p}^{(k)}\right), \qquad PI_{95\%} = [Q_{2.5}(Y), Q_{97.5}(Y)]$$

Where:

PI_95% = 95 percent prediction interval based on percentiles

Equation 11-6. Likelihood and posterior-style parameter updating.

$$L(\mathbf{p}) \propto \exp[-0.5\,\Phi(\mathbf{p})], \qquad f(\mathbf{p} \mid \mathbf{y}_{\mathrm{obs}}) \propto L(\mathbf{p})\,f(\mathbf{p})$$

If observed concentrations are $y_k^{obs}$and model outputs are $y_k^{mod}(\boldsymbol{\theta})$, with Gaussian residuals.

$$y_k^{obs} = y_k^{mod}(\boldsymbol{\theta}) + \varepsilon_k$$

$$\varepsilon_k \sim N(0, \sigma_\varepsilon^2)$$

Likelihood is:

$$p(D \mid \boldsymbol{\theta}, \sigma_\varepsilon) \propto \prod_{k=1}^{m} \exp\left[\; -\frac{\left(y_k^{obs} - y_k^{mod}(\boldsymbol{\theta})\right)^2}{2\sigma_\varepsilon^2}\right]$$

This is basis for Markov Chain Monte Carlo.

If posterior samples are $\boldsymbol{\theta}^{(1)}, \dots, \boldsymbol{\theta}^{(M)}$, then:

$$Y^{(m)} = \mathcal{M}(\boldsymbol{\theta}^{(m)})$$

and the collection of $Y^{(m)}$gives posterior predictive uncertainty across the entire cross-media pathway.

Where:

L(p) = likelihood of parameter set p

f(p | $\mathbf{y}_{\mathrm{obs}}$) = posterior parameter distribution

Equation 11-7. Medium-by-medium uncertainty Decomposition.

Atmospheric Uncertainty

$$U_{atmospheric} = f(Q, \mathrm{u}, K, v_d, P)$$

Deposition uncertainty

$$U_{deposition} = f(C_a, v_d, P, C_{rain})$$

Vadose zone uncertainty

$$U_{vadose\ zone} = f(K_d, K_{aw}, A_{aw}, \theta, \rho_b, v, D, L, \alpha, f_{pf})$$

Groundwater uncertainty

$$U_{groundwater} = f(R, D_{gw}, \mathbf{v}_{gw}, R_{gw}, \mu_{gw})$$

Then total uncertainty is propagated as:

$$U_{total} = U_{atm} \rightarrow U_{dep} \rightarrow U_{vadose\ zone} \rightarrow U_{gw}$$

Key assumptions

- The conceptual model correctly identifies whether PFAS are emitted primarily as gas, particles, aerosols, or mixed phases.
- The selected model class matches the spatial and temporal scale of the problem.
- Deposition velocities, scavenging coefficients, and phase-partition assumptions are reasonable effective parameters for the PFAS mixture being modeled.
- Cross-media transfer equations represent the dominant receiving-media processes at the scale of interest.
- Calibration and validation datasets are representative of the decision period and relevant to the output being defended.

Key limitations

- PFAS atmospheric chemistry remains less mature than criteria-pollutant chemistry; many model applications therefore rely on effective partitioning or transformation constructs rather than fully resolved mechanisms.
- Source characterization can dominate uncertainty. Stack tests, fugitives, and temporal emission profiles are often sparse or incomplete.
- Deposition data are much scarcer than air concentration data, making calibration and validation of deposition footprints difficult.
- Gas-particle partitioning for PFAS can vary with humidity, aerosol composition, chain length, functional group, and source process.
- Cross-media interpretations may be nonunique because soil or water PFAS can also arise from biosolids, wastewater, landfill leachate, groundwater discharge, or direct releases.

Conclusions

PFAS atmospheric deposition modeling is most defensible when it is framed as a mass-loading problem linked to soil, surface water, and groundwater, rather than as an air-only contouring exercise.

AERMOD, CALPUFF, CMAQ, CAMx, and SCICHEM each have a legitimate role, but the selected model must match the domain scale, atmospheric complexity, and chemistry needed for the decision. For near-field stack screening, AERMOD may be sufficient. For non-steady winds and deposition footprints, puff models are often superior. For regional transport and cumulative burden, Eulerian CTMs are the appropriate framework.

PFAS-specific uncertainty in emissions, partitioning, and deposition should be treated openly. The strongest technical white papers do not promise false mechanistic certainty; they show which assumptions matter, which outputs are robust, and which conclusions remain conditional.

AA GeoEnvironmental bottom line. The strongest PFAS atmospheric model is not the one with the most elaborate graphics. It is the one that uses the right governing equations for the right scale, converts air outputs into multimedia loading, and communicates uncertainty honestly.

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Appendix A. Equation Glossary and Core Symbol Definitions

The symbols used throughout this white paper follow standard atmospheric transport notation, but individual software packages may implement different variable names, dimensional conventions, or internal modules. The list below provides the most important recurring definitions used in this document.

C, C_i = Air concentration of PFAS or species i

Q = Emission rate

U, u = Wind speed or wind vector

K = Eddy diffusivity or diffusivity tensor

H = Effective stack height or Henry coefficient depending on context

σ_y, σ_z = Lateral and vertical plume spread parameters

M_p = Mass in a moving puff

V_d = Dry deposition velocity

Λ = Wet scavenging coefficient

J_{dep} = Total atmospheric deposition flux

K_p = Gas-particle partition coefficient

M_s, M_w = PFAS mass in soil or water control volume

q_r = Recharge rate

Φ = Objective function in calibration

J = Jacobian or sensitivity matrix

S_j = Sensitivity coefficient

C_p = Parameter covariance matrix

$PI\_95\%$ = 95 percent prediction interval

Appendix B. Emissions Characterization and Meteorological Inputs

The most influential input to a PFAS atmospheric model is often the emissions inventory rather than the transport solver. A defensible inventory should identify stack versus fugitive sources, operating schedule, control devices, chemical speciation, temperature, moisture, and whether releases are continuous, intermittent, or episodic. For many PFAS facilities, the dominant uncertainty is the chemical split among terminal ionic PFAS, neutral precursors, and particulate-bound material.

A useful source-term formulation for a stack release is:

Equation B-1. Emission-rate formulation based on activity and control.

$$Q_i(t) = EF_i(t)\,A(t)\,\eta_i(t)$$

Where:

$Q_i(t)$ = emission rate of species i at time t [M/T]

$EF_i(t)$ = emission factor or uncontrolled release rate per activity unit

$A(t)$ = activity rate or throughput

$\eta_i(t)$ = net fraction emitted after controls and capture

For measured stacks, emissions may instead be estimated directly from concentration and flow:

Equation B-2. Stack-emission-rate calculation from concentration and volumetric flow.

$$Q_i = C_s\,Q_v$$

Where:

C_s = stack concentration [M/L^3]

Q_v = stack volumetric flow rate [L^3/T]

If the source is fugitive over an area or building face, a practical relation is:

Equation B-3. Area-source emission formulation.

$$Q_A = E_A\,A_s$$

Where:

Q_A = area-source emission rate [M/T]

E_A = areal emission flux [M/L^2/T]

A_s = source area [L^2]

Meteorological representativeness is equally important. Near-field regulatory models depend on AERMET-style processing of surface and upper-air data or approved prognostic fields. Puff and Eulerian models rely on gridded meteorology that should be consistent with terrain, land-water contrasts, and the simulation period. In PFAS work, a poor meteorological year or an unrepresentative rain field can bias deposition predictions more than a moderate change in model formulation.

A simple precipitation-weighted average deposition over a simulation period is:

Equation B-4. Precipitation-weighted average deposition.

$$\bar{J}_{\text{dep},P} = \frac{\sum_t J_{\text{dep}}(t)\, P(t)}{\sum_t P(t)}$$

Where:

{J}{dep,P} = precipitation-weighted mean deposition flux

J_{dep}(t) = time-varying deposition flux

P(t) = time-varying precipitation depth or rate

Implementation note. When precipitation is the main deposition driver, modelers should scrutinize rain timing and location as carefully as wind direction. An otherwise good dispersion model can miss deposition hot spots if precipitation fields are wrong.

Appendix C. PFAS-Specific Atmospheric Partitioning and Transformation Considerations

PFAS atmospheric behavior is chemically heterogeneous. Neutral PFAS precursors may partition strongly to air and undergo oxidation or other transformation, whereas ionic PFAS often exhibit low volatility and may be emitted on particles or droplets. For that reason, PFAS atmospheric models commonly use effective partitioning, and reaction constructs rather than fully resolved chemistry for every compound.

A generic precursor-to-product transformation chain can be represented as:

Equation C-1. Lumped precursor-to-daughter transformation in air or in cloud/aqueous phases.

$$\frac{dC_p}{dt} = -k_p C_p, \qquad \frac{dC_d}{dt} = Y_{pd}\, k_p C_p - k_d C_d$$

Where:

C_p = precursor concentration

C_d = daughter concentration

k_p = effective precursor loss rate [1/T]

k_d = effective daughter loss rate [1/T]

Ypd = effective yield from precursor to daughter

A two-phase deposition-weighted concentration can be written as:

Equation C-2. Effective concentration combining gas and particle fractions.

$$C_{\text{eff}} = f_g C_g + f_p C_p$$

Where:

C_{eff} = effective concentration for deposition or exposure calculations

f_g, f_p = gas- and particle-fraction weights

C_g, C_p = gas- and particle-phase concentrations

If particle settling is important, a simple deposition relation is:

Equation C-3. Deposition velocity decomposed into aerodynamic transfer and settling.

$$V_d = V_a + v_g$$

Where:

V_d = total deposition velocity

V_a = non-settling transfer component

v_g = gravitational settling velocity

For spherical particles in the Stokes regime, settling velocity may be approximated by:

Equation C-4. Stokes-law settling velocity.

$$v_g = \frac{(\rho_p - \rho_a)\, g\, d_p^2\, C_c}{18\, \mu}$$

Where:

ρ_p = particle density

ρ_a = air density

g = gravitational acceleration

d_p = particle diameter

Cc = Cunningham slip correction factor

μ = dynamic viscosity of air

These equations are not PFAS-specific laws; they are physically standard transport constructs applied to PFAS according to the phase and particle assumptions selected for the case. The analyst should therefore state clearly whether a given PFAS is being represented as gaseous, particle-associated, or split across both phases, and whether any atmospheric transformation is modeled mechanistically or as an effective first-order term.

Where source information is limited, scenario analysis should be used. A common defensible approach is to run three cases: all-gas, all-particle, and split-phase emissions using literature-supported bounds. If predicted deposition conclusions are similar across the scenarios, the decision is more robust.

PFAS-specific caution. Many PFAS applications appear numerically precise but are chemically underdetermined. It is usually better to bracket gas-particle and precursor assumptions transparently than to present one highly specific chemistry case without support.

Appendix D. Model Selection Workflow and Expert Review Checklist

A practical expert review starts with scale. If the source-receptor distance is short, winds are reasonably stationary over each averaging period, and the need is near-field screening, a plume model may be appropriate. If complex coastal or terrain flows control the outcome, a puff model is often more defensible. If the problem is cumulative annual deposition over a broad region, an Eulerian chemistry-transport model is typically required.

The model-selection decision can be expressed conceptually as:

Equation D-1. Conceptual model-selection objective.

$$M^* = \underset{M}{\operatorname{argmin}}\{\mathrm{Risk}(M,S,P,D) + \mathrm{Cost}(M)\}$$

Where:

M* = preferred model class

M = candidate model class

S = spatial and temporal scale of the problem

P = process complexity required

D = decision consequence

Cost(M) = resource and data cost of model class M

A practical source-apportionment fraction from atmospheric deposition is:

Equation D-2. Source-attributable deposition fraction.

$$f_{\mathrm{atm}} = \frac{J_{\mathrm{dep,source}}}{J_{\mathrm{dep,total}}}$$

Where:

$\mathbf{f_{atm}}$ = fraction of total deposition attributable to the modeled source

$\mathbf{J_{dep,source}}$ = source-attributable deposition flux

$\mathbf{J_{dep,total}}$ = total deposition flux including background or other sources

A corresponding soil-burden attributable fraction is:

Equation D-3. Soil burden attributable to atmospheric loading.

$$f_{\text{soil}} = \frac{M_{\text{soil,atm}}}{M_{\text{soil,total}}}$$

Where:

$M_{\text{soil,atm}}$ = soil PFAS mass attributable to atmospheric deposition

$M_{\text{soil,total}}$ = total measured or estimated soil PFAS mass

Reviewers should also ask whether deposition is materially distinguishable from background. Regional and global atmospheric transport means that low PFAS concentrations in soil or rainwater may exist even away from obvious local emitters. Therefore, comparison to upwind or reference conditions, model background treatment, and multi-source runs are important parts of defensibility.

A practical checklist for an AA GeoEnvironmental-style review includes: (1) Is atmospheric deposition likely to matter relative to other pathways? (2) Does the emissions inventory distinguish species and phase appropriately? (3) Is the selected model class matched to the source-receptor scale? (4) Are deposition and receiving-media loading outputs reported? (5) Is validation tied to independent data? (6) Are uncertainty ranges provided for emissions and phase assumptions?

Review standard. An atmospheric PFAS model is strongest when it can survive a cross-examination on source term, model choice, deposition treatment, and background attribution—not just when it reproduces a few monitoring values.

Appendix E. Data Requirements, QA/QC, and Minimum Technical Documentation

A publishable or litigation-resilient PFAS atmospheric model should preserve complete metadata for emissions, meteorology, terrain/land use, receptor grids, chemical speciation, deposition parameters, calibration targets, and QA/QC checks. Reproducibility is part of defensibility.

At minimum, technical documentation should include source coordinates, release geometry, stack parameters, process schedule, emissions basis, meteorological years used, precipitation source, receptor strategy, deposition options, gas-particle assumptions, sensitivity scenarios, and comparison plots against measured data. Where deposition is the main prediction, maps of cumulative dry, wet, and total deposition should be reported alongside annual areal loading summaries.

A minimum mass-balance QA/QC check for Eulerian simulations may be stated as:

Equation E-1. Illustrative mass-balance closure check.

$$\text{Mass\_error} = \frac{M_{\text{initial}} + M_{\text{emitted}} - M_{\text{remaining}} - M_{\text{deposited}} - M_{\text{outflow}} - M_{\text{reacted}}}{M_{\text{emitted}}}$$

Where:

Mass_error = relative mass-balance residual

$M_{initial}$ = initial mass in domain

$M_{emitted}$ = mass emitted during the run

$M_{remaining}$ = mass remaining in domain at end of run

$M_{deposited}$ = mass deposited to surfaces

$M_{outflow}$ = mass that advected out of the domain

$M_{reacted}$ = mass lost to reactions or other sinks

Caveat. Large unexplained mass imbalance, unrealistic deposition discontinuities at nested-grid boundaries, or strong dependence on one arbitrary phase assumption are all warnings that the simulation needs additional scrutiny.