AA GeoEnvironmental Technical White Paper
3-D Groundwater Flow and Contaminant Transport Modeling

Governing Equations, Calibration with PEST, Sensitivity, Validation, Uncertainty, Assumptions, and Limitations

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Purpose. This white paper provides a detailed, practice-oriented mathematical and technical framework for three-dimensional groundwater modeling suitable for conceptual site model development, forensic review, remedial design support, and independent technical evaluation by AA GeoEnvironmental.

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Executive Summary

Three-dimensional groundwater models quantify the spatial and temporal evolution of hydraulic heads, groundwater flows, pathlines, capture zones, plume migration, and contaminant mass flux. In professional practice, a model is only as valid as its conceptual site model, which includes governing equations, boundary conditions, parameterization, calibration technique, and uncertainty analysis.

This white paper presents the fundamental mathematical equations and practical interpretations required for a thorough groundwater model review. It discusses Darcy flow, continuity, confined and unconfined storage, anisotropy, boundary conditions, advection-dispersion-reaction transport, sorption and decay, dual-domain processes, particle tracking, PEST-based inverse calibration, sensitivity analysis, model predictive validation, uncertainty analysis, and common red flags that reduce model reliability.

The key conclusion is simple: a 3-D groundwater model is not persuasive because it is enormous, expensive, or visually appealing. It is convincing when the mathematical formulation matches the site physics, calibration targets are relevant to the prediction of interest, sensitivity is understood, limitations are revealed, and uncertainty is quantified rather than concealed.

> Three-dimensional groundwater modeling should be used to illuminate the decision, not to instill false confidence. The most effective models are transparent about what they can and cannot resolve.

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1. Purpose, Scope, and Conceptual Model Foundations

Three-dimensional groundwater modeling is used to depict subsurface systems in which flow and contaminant transport change horizontally, vertically, and temporally. Typical applications include water-supply capture zone analysis, plume delineation, remedial design, monitored natural attenuation evaluation, pumping-test interpretation, mass-flux calculation, saltwater intrusion study, and regulatory or litigation support.

A robust model starts with a conceptual site model rather than a grid. The conceptual model should identify hydrostratigraphic units, hydraulic connectivity, recharge and discharge processes, aquifer heterogeneity, storage mechanisms, hydraulic boundaries, contaminant sources and release histories, pathways, receptors, and decision-relevant predictions. A three-dimensional model is required when the site has irregular source geometry, anisotropic flow, layered heterogeneity, rivers or drains that vary in plan view, partial-penetration effects, varying pumping stresses, or multidirectional plume migration.

Common conceptual simplifications include equivalent porous media for fractured or karst systems, hydrostratigraphic zonation, areal recharge as a flux boundary, and effective dispersivities that represent persistent heterogeneity. These simplifications are valid, but only when their implications for interest prediction are explicitly considered.

> **Professional interpretation.** The most prevalent failure in groundwater modeling is not the solver. It is an insufficient conceptual site model that is then rendered with false numerical precision.

2. Governing Equations for 3-D Groundwater Flow

Groundwater flow models are founded on Darcy's law and the principle of conservation of mass. The combination of these elements results in the three-dimensional flow equation utilized in MODFLOW-class simulators and associated numerical codes.

Equation 2-1. Darcy flux in vector form.

$$\mathbf{q} = -\mathbf{K}\nabla h$$

Where:

- **q** = specific discharge or Darcy flux vector [L/T]
- **K** = hydraulic-conductivity tensor [L/T]
- **∇h** = hydraulic-head gradient [-]

In anisotropic media, hydraulic conductivity is better represented as a tensor rather than a scalar:

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Equation 2-2. Hydraulic-conductivity tensor

$$\mathbf{K} = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix}$$

Where:

- $\mathbf{K_{xx} \ldots K_{zz}}$ = principal and cross-conductivity components [L/T]

Combining Darcy's law with mass conservation yields the transient confined flow equation in tensor form:

Equation 2-3. Three-dimensional transient groundwater-flow equation for a saturated confined system.

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (\mathbf{K}\nabla h) + W$$

Where:

- **Ss** = specific storage [1/L]
- **h** = hydraulic head [L]
- **t** = time [T]
- **∇ · (K ∇h)** = divergence of conductive flux [1/T]
- **W** = volumetric flux per unit volume representing sources and sinks [1/T]

Expanded in Cartesian coordinates, the anisotropic form becomes:

Equation 2-4. Expanded diagonal-tensor form for orthogonal principal directions.

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) + W$$

Where:

x, y, z = spatial coordinates [L]

$\mathbf{K_{xx}, K_{yy}, K_{zz}}$ = directional hydraulic conductivity [L/T]

For water-table systems, specific yield often dominates storage, and a common practical approximation is:

Equation 2-5. Practical unconfined approximation for small water-table fluctuations.

$$S_y \frac{\partial h}{\partial t} = \nabla \cdot (K_{sat}\, b\, \nabla h) + W$$

Where:

Sy = specific yield [-]

Ksat = saturated hydraulic conductivity [L/T]

b = saturated thickness [L]

The general volumetric continuity equation can also be written:

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Equation 2-6. Mass continuity equation for variable density or compressible formulations.

$$\frac{\partial(\rho\theta)}{\partial t} + \nabla \cdot (\rho \mathbf{q}) = Q_m$$

Where:

ρ = fluid density [M/L³]

θ = effective porosity or fluid content [-]

Qm = mass source/sink term [M/L³/T]

Most site-scale freshwater models simplify to constant density, but variable-density formulations become important in coastal aquifers, brine plumes, and thermal or salinity gradients.

Real-world meaning. Groundwater flow in 3-D is driven by head gradients, modulated by anisotropy and storage, and reshaped by boundaries and stresses. The governing equation is simple to write and difficult to parameterize correctly.

Boundary and initial conditions are as important as the differential equation itself. Standard forms include prescribed head, prescribed flux, and head-dependent flux boundaries.

Equation 2-7. Dirichlet (specified-head) boundary condition.

$$h = h_B \quad \text{on } \Gamma_h$$

Where:

$\mathbf{h_B}$ = specified boundary head [L]

$\mathbf{\Gamma_h}$ = head boundary portion of the domain

Equation 2-8. Neumann (specified-flux) boundary condition.

$$-\mathbf{n} \cdot \mathbf{q} = q_B \quad \text{on } \Gamma_q$$

Where:

n = outward unit normal vector [-]

$\mathbf{q_B}$ = specified boundary flux [L/T]

$\mathbf{\Gamma_q}$ = flux boundary portion of the domain

Equation 2-9. Cauchy or head-dependent flux boundary condition.

$$-\mathbf{n} \cdot \mathbf{q} = C_b\,(h - h_R) \quad \text{on } \Gamma_c$$

Where:

$\mathbf{C_b}$ = boundary conductance [1/T]

$\mathbf{h_R}$ = reference or stage head [L]

$\mathbf{\Gamma_c}$ = head-dependent boundary portion of the domain

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3. Governing Equations for 3-D Contaminant Transport

The standard solute-transport equation for dissolved contaminants in groundwater is the advection-dispersion-reaction equation. The general form used in MT3DMS, MT3D-USGS, and MODFLOW 6 GWT-type models is:

Equation 3-1. General three-dimensional advection-dispersion-reaction equation.

$$\frac{\partial(\theta C)}{\partial t} + \rho_b \frac{\partial S}{\partial t} = \nabla \cdot (\theta \mathbf{D} \nabla C) - \nabla \cdot (\mathbf{q} C) + q_s C_s - \lambda_w \theta C - \lambda_s \rho_b S + R$$

Where:

C = dissolved concentration [M/L^3]

θ = effective porosity or mobile water content [-]

ρb = bulk density [M/L^3]

S = sorbed concentration [M/M]

D = hydrodynamic-dispersion tensor [L^2/T]

q = Darcy flux vector [L/T]

qs = volumetric fluid source/sink term [1/T]

Cs = concentration associated with source/sink water [M/L^3]

λ_w = first-order aqueous decay coefficient [1/T]

λ_s = first-order decay coefficient for sorbed mass [1/T]

R = other reaction terms [$M/L^3/T$]

The transport equation may be expanded into advection, dispersion, retardation, and reaction sub-processes. The advective flux is simply the product of Darcy flux and concentration, while the dispersive flux combines mechanical dispersion with molecular diffusion.

Equation 3-2. Average linear groundwater velocity.

$$\mathbf{v} = \frac{\mathbf{q}}{\theta}$$

Where:

v = pore-water or seepage velocity vector [L/T]

Equation 3-3. Common hydrodynamic-dispersion tensor for porous media.

$$D_{ij} = \alpha_T |\mathbf{v}|\, \delta_{ij} + (\alpha_L - \alpha_T) \frac{v_i v_j}{|\mathbf{v}|} + \tau D_m\, \delta_{ij}$$

Where:

D_{ij} = component of the dispersion tensor [L^2/T]

αL = longitudinal dispersivity [L]

αT = transverse dispersivity [L]

|**v**| = magnitude of seepage velocity [L/T]

δij = Kronecker delta [-]

τ = tortuosity factor [-]

Dm = molecular diffusion coefficient in water [L^2/T]

For linear equilibrium sorption, the standard isotherm is:

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Equation 3-4. Linear sorption isotherm.

$$S = K_d C$$

Where:

Kd = distribution coefficient [L³/M]

This leads to the familiar retardation factor:

Equation 3-5. Retardation factor for linear equilibrium sorption.

$$R_f = 1 + \frac{\rho_b K_d}{\theta}$$

Where:

R = retardation factor [-]

A nonlinear Freundlich form is often used when sorption is concentration dependent:

Equation 3-6. Freundlich sorption isotherm.

$$S = K_f C^N$$

Where:

$\mathbf{K_f}$ = Freundlich coefficient

N = Freundlich exponent [-]

First-order decay in water is written as:

Equation 3-7. First-order aqueous decay.

$$\frac{\partial C}{\partial t} = -\lambda_w C$$

Where:

λ = first-order decay constant [1/T]

For sequential reactions, common in chlorinated-solvent chains or radionuclide decay series, production and loss can be written as:

Equation 3-8. Generic daughter production and loss term.

$$R_i = Y_i \lambda_p C_p - \lambda_i C_i$$

Where:

Ri = net reaction term for species i [M/L³/T]

Yi = yield coefficient [-]

λp = parent transformation coefficient [1/T]

Cp = parent concentration [M/L³]

Ci = daughter concentration [M/L³]

Dual-domain or mobile-immobile formulations are often important in fractured, saprolitic, or low-permeability settings with matrix diffusion or back-diffusion:

Equation 3-9. Mobile-domain transport in a dual-domain system.

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$$\theta_m \frac{\partial C_m}{\partial t} + \rho_b \frac{\partial S_m}{\partial t} = \nabla \cdot (\theta_m D_m \nabla C_m) - \nabla \cdot (\mathbf{q}_m C_m) - \alpha_{ex}(C_m - C_{im})$$

Where:

- θ_m = mobile-domain porosity [-]
- C_m = mobile-domain concentration [M/L³]
- S_m = mobile-domain sorbed concentration [M/M]
- **αex** = mass-exchange coefficient [1/T]
- C_{im} = immobile-domain concentration [M/L³]

Equation 3-10. Immobile-domain exchange equation.

$$\theta_{im} \frac{dC_{im}}{dt} + \rho_b \frac{dS_{im}}{dt} = \alpha_{ex}(C_m - C_{im})$$

Where:

- θ_{im} = immobile-domain porosity [-]
- S_{im} = immobile-domain sorbed concentration [M/M]

Professional interpretation. In transport modeling, the prediction of interest controls which processes must be represented. Capture-zone or travel-time questions may only need advective particle tracking. Mass-flux, cleanup-time, attenuation, or source-decay questions almost always require a full transport equation.

4. Numerical Implementation and Model Construction Choices

The governing equations are not solved analytically for most real sites. They are discretized in space and time using finite-difference, finite-volume, or finite-element methods. MODFLOW and many associated transport codes use control-volume finite-difference formulations that conserve water and mass at the cell scale.

Spatial discretization divides the model domain into cells or elements. Temporal discretization divides the simulation into stress periods and time steps. The chosen discretization affects stability, mass balance, parameter zonation, runtime, and the numerical diffusion observed in the solution. The grid should be fine enough to resolve hydraulic gradients, pumping stresses, source areas, and compliance boundaries, but not so fine that the model becomes numerically unstable, poorly parameterized, or too costly to analyze probabilistically.

Common numerical diagnostics include the cell Peclet number and Courant number:

Equation 4-1. Cell Peclet number.

$$Pe = \frac{v\,\Delta x}{D}$$

Where:

- **Δl** = representative cell dimension [L]
- **D** = dispersion coefficient in the direction of flow [L²/T]

Equation 4-2. Courant number.

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$$Co = \frac{v\,\Delta t}{\Delta x}$$

Where:

Δt = time-step length [T]

Very large Peclet numbers can indicate excessive numerical dispersion or oscillation risk in advection-dominated transport. Excessive Courant numbers can indicate time stepping that is too coarse for the transport process being simulated.

Mass-balance checks remain essential. A simple percent discrepancy formulation is:

Equation 4-3. Generic groundwater mass-balance discrepancy metric.

$$MBE = \frac{\sum Q_{in} - \sum Q_{out} - \Delta S}{\sum Q_{in}} \times 100\%$$

Where:

Inflows = sum of all inflow rates [L^3/T]

Outflows = sum of all outflow rates [L^3/T]

$\mathbf{\Delta_{Storage}}$ = rate of storage change [L^3/T]

> **Why this matters.** A visually smooth plume can still be numerically wrong. Coarse grids, poor time stepping, and unstable advection solutions can create elegant but misleading model output.

5. Calibration with PEST and Related Inverse Methods

Calibration estimates parameter values so simulated heads, flows, and concentrations are reasonably consistent with observations. Trial-and-error calibration remains common, but highly parameterized inverse methods are generally more transparent and repeatable when used carefully.

Equation 5-1. Weighted least-squares objective function.

$$\Phi(\mathbf{p}) = \sum_{i=1}^{n} w_i \left[y_i^{obs} - y_i(\mathbf{p})\right]^2$$

Where:

Φ(p) = objective function value [-]

p = parameter vector

wi = observation weight

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

yi(p) = simulated counterpart for target i

Observation weights are commonly derived from variance or from professional judgment about relative reliability:

Equation 5-2. Variance-based observation weight.

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

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Where:

σ_i^2 = variance of observation error for target i

Regularization is commonly added to stabilize high-dimensional inverse problems:

Equation 5-3. Composite objective function with regularization.

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

Where:

Φ_{obs} = fit-to-observation component [-]

μ = regularization weight [-]

Φ_{reg} = regularization penalty [-]

Equation 5-4. Preferred-value or Tikhonov regularization term.

$$\Phi_{reg} = \sum_{j=1}^{m} \left(\frac{p_j - p_{j,prior}}{\sigma_{p_j}} \right)^2$$

Where:

$p_{j,prior}$ = preferred or prior parameter value

σ_{pj} = allowable deviation or prior uncertainty

The parameter-update step in a Gauss-Newton or Levenberg-Marquardt framework is typically written:

Equation 5-5. Damped least-squares parameter-update equation.

$$(\mathbf{J}^T\mathbf{W}\mathbf{J} + \lambda\mathbf{I})\,\Delta\mathbf{p} = \mathbf{J}^T\mathbf{W}\mathbf{r}$$

Where:

J = Jacobian sensitivity matrix

W = diagonal weighting matrix

λ = damping factor

I = identity matrix

Δp = parameter update vector

r = residual vector

Residuals are simply:

Equation 5-6. Residual for observation i.

$$e_i = y_i^{obs} - y_i(\mathbf{p})$$

Where:

e_i = residual for observation i

Equation 5-7. Weighted residual.

$$e_{w,i} = \sqrt{w_i}\,e_i$$

Where:

$e_{w,i}$ = weighted residual for observation i

Common fit statistics include:

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Equation 5-8. Root mean square error.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(y_i^{obs} - y_i\right)^2}$$

Where:

n = number of observations

Equation 5-9. Mean absolute error.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|y_i^{obs} - y_i\right|$$

Equation 5-10. Percent bias.

$$PBIAS = 100\,\frac{\sum_{i=1}^{n}\left(y_i - y_i^{obs}\right)}{\sum_{i=1}^{n} y_i^{obs}}$$

Equation 5-11. Nash-Sutcliffe efficiency.

$$NSE = 1 - \frac{\sum_{i=1}^{n}\left(y_i^{obs} - y_i\right)^2}{\sum_{i=1}^{n}\left(y_i^{obs} - \bar{y}^{obs}\right)^2}$$

Where:

$\bar{y}_{obs}$ = mean observed value

For highly parameterized models, PEST and PEST++ are particularly valuable because they support automated parameter estimation, singular-value decomposition, and calibration-constrained uncertainty analysis. In practice, however, no optimizer can rescue a poor conceptual model. The objective function measures fit to data; it does not certify physical truth.

> **Calibration principle.** Calibrate to the prediction of interest. If the decision depends on river capture, include heads and streamflow gains or losses. If the decision depends on plume travel time, include concentrations, gradients, and source behavior, not just hydraulic heads.

6. Sensitivity Analysis and Validation

Sensitivity analysis measures how strongly model outputs respond to parameter changes. It is essential for parameter estimation, data-worthy analysis, and accurate interpretation of calibration results

Equation 6-1. Local sensitivity of output Y to parameter pj.

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

Where:

Y = selected model output or prediction

Equation 6-2. Dimensionless local sensitivity.

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

Equation 6-3. Composite scaled sensitivity.

$$CSS_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{\partial y_i}{\partial p_j}\,p_j\sqrt{w_i}\right)^2}$$

Where:

CSS_j = composite scaled sensitivity for parameter j

Global sensitivity methods are often more informative for nonlinear models with interacting parameters.

Equation 6-4. Morris elementary effect.

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

Where:

EEi = elementary effect of factor i

X = vector of model factors

Δ = factor perturbation

Equation 6-5. Mean absolute elementary effect.

$$\mu_i^* = \frac{1}{r}\sum_{j=1}^{r}\left|EE_{i,j}\right|$$

Where:

r = number of Morris trajectories

Equation 6-6. Standard deviation of elementary effects.

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

Equation 6-7. Variance decomposition used in Sobol analysis.

$$Var(Y) = \sum_i V_i + \sum_{i<j} V_{ij} + \cdots + V_{12\ldots k}$$

Where:

V_i = first-order variance contribution

V_{ij} = second-order interaction contribution

Equation 6-8. First-order Sobol index.

$$S_i = \frac{V_i}{Var(Y)}$$

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Where:

Si = main-effect Sobol sensitivity index for factor i

Equation 6-9. Total-effect Sobol index.

$$S_{T_i} = 1 - \frac{Var_{X_{\sim i}}\left(E_{X_i}[Y \mid X_{\sim i}]\right)}{Var(Y)}$$

Where:

STi = total-effect Sobol sensitivity index

Model validation in environmental systems is better viewed as corroboration than proof. Because real groundwater systems are open and partially observed, a calibrated model cannot be declared universally valid. The stronger practice is to test the model against withheld observations, alternate stress periods, independent datasets, or post-audit conditions and then judge whether the model is adequate for the prediction at issue.

Useful validation or corroboration statistics include withheld-data RMSE, predictive bias, temporal split-sample tests, spatial holdout tests, and post-audit comparison to conditions observed after the original calibration period. A simple withheld-data RMSE is:

Equation 6-10. Validation RMSE on independent observations.

$$RMSE_{val} = \sqrt{\frac{1}{n_{val}} \sum_{i=1}^{n_{val}} \left(y_{i,val}^{obs} - y_{i,val}\right)^2}$$

Where:

m = number of withheld observations

Equation 6-11. Split-Sample Validation.

Split-Sample Validation

$$\mathbf{p}^* = \arg\min_{\mathbf{p}} \quad \Phi_{cal}(\mathbf{p})$$

With calibration objective:

$$\Phi_{cal}(\mathbf{p}) = \sum_{i=1}^{n_{cal}} w_i \left(y_i^{obs} - y_i^{sim}(\mathbf{p})\right)^2$$

Validation with independent data is then evaluated:

$$\Phi_{val}(\mathbf{p}^*) = \sum_{j=1}^{n_{val}} w_j \left(y_j^{obs} - y_j^{sim}(\mathbf{p}^*)\right)^2$$

Where:

- $\mathbf{p}$= parameter vector
- $\mathbf{p}^*$= calibrated parameter set
- Φ_{cal}= calibration objective function
- Φ_{val}= validation objective function

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- n_{cal}= number of calibration observations
- n_{val}= number of validation observations

Important caution. A model can be well calibrated and poorly predictive if it was tuned to the wrong targets, if forcing data are wrong, or if the model structure is missing a controlling process such as leakage, matrix diffusion, or changing source strength.

7. Uncertainty Analysis and Prediction Defensibility

Uncertainty analysis quantifies how much confidence can be placed in a model prediction after considering parameter uncertainty, observation error, scenario uncertainty, and structural simplification.

Equation 7-1. Linearized parameter covariance matrix.

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

Where:

Cp = parameter covariance matrix

s² = estimated residual variance

Equation 7-2. Residual variance estimate at the calibrated optimum.

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

Where:

p* = calibrated or optimal parameter vector

m = number of estimated parameters

Equation 7-3. Standard error of parameter pj.

$$SE(p_j) = \sqrt{C_{p,jj}}$$

Equation 7-4. First-order prediction variance.

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

Where:

Z = selected prediction

gp = gradient vector of the prediction with respect to parameters

Equation 7-5. Prediction standard deviation.

$$\sigma_Z = \sqrt{Var(Z)}$$

Equation 7-6. Likelihood-style weighting based on the objective function.

$$L(\mathbf{p}) \propto \exp\left(-\frac{1}{2}\Phi(\mathbf{p})\right)$$

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Where:

L(p) = likelihood or relative plausibility of parameter set p

Equation 7-7. Posterior-style updating of parameter uncertainty.

$$f\left(\mathbf{p} \mid \mathbf{y}^{obs}\right) \propto L(\mathbf{p})\, f(\mathbf{p})$$

Where:

$f(p|y^{obs})$ = posterior parameter distribution

f(p) = prior parameter distribution

Equation 7-8. Monte Carlo or Latin Hypercube parameter sampling.

$$\mathbf{p}^{(k)} \sim f_{\mathbf{p}}(\mathbf{p}), \qquad k = 1, \dots, N$$

Where:

N = number of realizations

Equation 7-9. Model response for realization k.

$$Y^{(k)} = f\left(\mathbf{p}^{(k)}\right)$$

Where:

Y(k) = prediction generated by realization k

Equation 7-10. Percentile-based 95% prediction interval.

$$PI_{95\%} = [Q_{2.5}(Y), Q_{97.5}(Y)]$$

Where:

Q2.5, Q97.5 = 2.5th and 97.5th percentiles

Equation 7-11. Null-space Monte Carlo concept.

$$\mathbf{p}^{(k)} = \mathbf{p}^{*} + \mathbf{V}_n \mathbf{a}^{(k)}$$

Where:

V_n = basis vectors spanning the null space

a(k) = random coefficients for realization k

Equation 7-12. Practical decomposition of total predictive uncertainty.

$$Var_{total}(Z) = Var_{param}(Z) + Var_{obs}(Z) + Var_{scenario}(Z) + Var_{structure}(Z)$$

Where:

Var_{param} = parameter uncertainty contribution

Var_{obs} = observation-error contribution

$Var_{scenario}$ = scenario or future-stress uncertainty

$Var_{structure}$ = model-structure uncertainty

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The most professional uncertainty workflow is calibrated, prediction-focused, and transparent. It shows how uncertain the decision metric remains after reasonable parameter adjustment, alternate conceptual models, plausible future stresses, and data limitations are considered.

> **Decision relevance.** For remedy selection, the useful output is not only the calibrated plume map. It is the range of plausible travel times, concentrations, capture efficiencies, or cleanup durations that remain consistent with the data and model assumptions.

8. Assumptions and Limitation

All groundwater models simplify reality. The question is whether the simplifications are appropriate for the decision being supported.

Common assumptions include approximate Darcy flow through a representative porous medium; hydrostratigraphic units that can be represented with effective properties; source and sink stresses that are known or can be approximated; and reaction terms that reasonably represent the chemistry at the modeling scale. Each assumption should be stated explicitly and tested for importance when practical.

Key limitations include parameter nonuniqueness, sparse data, uncertain recharge, uncertain source history, uncertain boundary conditions, scale effects between field tests and model cells, numerical dispersion, and structural uncertainty. Heterogeneity below the grid scale is almost always present and often only partially represented through effective parameters such as dispersivity or zoned conductivity.

> **AA GeoEnvironmental review lens.** The strongest technical review question is not "Does this model run?" It is "Does this model resolve the decision-relevant physics, and are the uncertainties honestly communicated?"

9. Conclusions and Recommendations

A detailed 3-D groundwater model can be an exceptionally powerful decision-support tool when it is built around a sound conceptual site model, mathematically appropriate governing equations, and a calibration and uncertainty strategy tied to the actual prediction of interest.

For groundwater flow, the core equations are Darcy's law, continuity, and the transient 3-D flow equation with appropriate storage and boundary conditions. For contaminant transport, the core equation is the 3-D advection-dispersion-reaction equation supplemented as necessary by sorption, decay, dual-domain exchange, matrix diffusion, or other reaction terms.

PEST-based calibration and related inverse methods can improve transparency and reproducibility, but they do not replace conceptual judgment. Sensitivity analysis should be used to identify which parameters matter, validation or corroboration should be directed toward the intended prediction, and uncertainty should be shown explicitly through covariance methods, Monte Carlo simulation, null-space approaches, or structured scenario analysis.

The most defensible groundwater white papers are those that state assumptions clearly, acknowledge limitations, identify red flags proactively, and make the model answer the right question at the right scale.

> **Final message.** A groundwater model earns credibility through alignment of physics, data, calibration, and uncertainty - not through complexity alone.

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References

Anderson, M. P., Woessner, W. W., & Hunt, R. J. (2015). Applied groundwater modeling: Simulation of flow and advective transport (2nd ed.). Academic Press.

Bear, J. (1972). Dynamics of fluids in porous media. Elsevier.

Bedekar, V., Morway, E. D., Langevin, C. D., & Tonkin, M. J. (2016). MT3D-USGS version 1: A U.S. Geological Survey release of MT3DMS updated with new and expanded transport capabilities for use with MODFLOW. U.S. Geological Survey Techniques and Methods 6-A53.

Campolongo, F., Cariboni, J., & Saltelli, A. (2007). An effective screening design for sensitivity analysis of large models. Environmental Modelling & Software, 22(10), 1509-1518.

Doherty, J. (2005). PEST: Model-independent parameter estimation manual (4th ed.). Watermark Numerical Computing.

Doherty, J. and Simmons, C.T., 2013. Groundwater modelling in decision support: reflections on a unified conceptual framework. *Hydrogeology Journal* 21: 1531–1537

Doherty, J. (2015). *Calibration and uncertainty analysis for complex environmental models*. Watermark Numerical Computing.

Doherty, J. and Moore, C., 2019. Decision support modeling: data assimilation, uncertainty quantification and strategic abstraction. *Groundwater* 58(3) 327-337 doi: 10.1111/gwat.12969.

Domenico, P. A., & Schwartz, F. W. (1998). Physical and chemical hydrogeology (2nd ed.). Wiley.
Fetter, C. W. (2018). Applied hydrogeology (5th ed.). Waveland Press.

Freeze, R. A., & Cherry, J. A. (1979). Groundwater. Prentice Hall.

Harbaugh, A. W. (2005). MODFLOW-2005, the U.S. Geological Survey modular ground-water model: The Ground-Water Flow Process. U.S. Geological Survey Techniques and Methods 6-A16.

Hill, M. C., & Tiedeman, C. R. (2007). Effective groundwater model calibration: With analysis of data, sensitivities, predictions, and uncertainty. Wiley.

Hill, M. C. (1998). Methods and guidelines for effective model calibration. *U.S. Geological Survey Water-Resources Investigations Report 98-4005*. U.S. Geological Survey (water.usgs.gov).

Hill, M. C., Banta, E. R., Harbaugh, A. W., & Anderman, E. R. (2000). MODFLOW-2000, the U.S. Geological Survey modular ground-water model—User guide to the Observation, Sensitivity, and Parameter-Estimation Processes and three post-processing programs. *U.S. Geological Survey Open-File Report 00-184*. U.S. Geological Survey (pubs.usgs.gov).

Hill, M. C., & Tiedeman, C. R. (2007). *Effective groundwater model calibration: With analysis of data, sensitivities, predictions, and uncertainty*. Hoboken, NJ: John Wiley & Sons. (books.google.com)

Hughes, J. D., Langevin, C. D., & Banta, E. R. (2017). Documentation for the MODFLOW 6 framework. U.S. Geological Survey Techniques and Methods 6-A57.

Konikow, L. F., & Bredehoeft, J. D. (1992). Ground-water models cannot be validated. *Advances in Water Resources, 15*(1), 75-83. https://doi.org/10.1016/0309-1708(92)90033-X.

Langevin, C. D., Hughes, J. D., Banta, E. R., Niswonger, R. G., Panday, S., & Provost, A. M. (2017). Documentation for the MODFLOW 6 Groundwater Flow Model. U.S. Geological Survey Techniques and Methods 6-A55.

Langevin, C. D., Thorne, D. T., Dausman, A. M., Sukop, M. C., & Guo, W. (2008). SEAWAT version 4: A computer program for simulation of multi-species solute and heat transport. U.S. Geological Survey Techniques and Methods 6-A22.

McDonald, M. G., & Harbaugh, A. W. (1988). A modular three-dimensional finite-difference ground-water flow model. U.S. Geological Survey Techniques of Water-Resources Investigations, Book 6, Chapter A1.

Moriasi, D. N., Gitau, M. W., Pai, N., & Daggupati, P. (2015). Hydrologic and water quality models: Performance measures and evaluation criteria. *Transactions of the ASABE, 58*(6), 1763-1785. https://doi.org/10.13031/trans.58.10715

Morris, M. D. (1991). Factorial sampling plans for preliminary computational experiments. Technometrics, 33(2), 161-174.
Mualem, Y. (1976). A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resources Research, 12(3), 513-522.

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National Ground Water Association. (2016). Review of Applied Groundwater Modeling: Simulation of Flow and Advective Transport, 2nd edition. Groundwater, 54(3), 486-487.

PEST Homepage. (n.d.). PEST and PEST++ documentation and downloads. Retrieved March 20, 2026, from https://pesthomepage.org/

Pollock, D. W. (2016). User guide for MODPATH version 7: A particle-tracking model for MODFLOW. U.S. Geological Survey Open-File Report 2016-1086.

Poeter, E. P., & Hill, M. C. (1999). UCODE, a computer code for universal inverse modeling. Computers & Geosciences, 25(4), 457-462.

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., & Tarantola, S. (2008). Global Sensitivity Analysis: The Primer. John Wiley & Sons. ISBN: 9780470725177.

Sanders, M. J., Panday, S., Langevin, C. D., Niswonger, R. G., Provost, A. M., & Hughes, J. D. (2022). Documentation for the MODFLOW 6 Groundwater Transport Model. U.S. Geological Survey Techniques and Methods 6-A61.

Sobol, I. M. (2001). Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Mathematics and Computers in Simulation, 55(1-3), 271-280.

Tiedeman, C. R., & Hill, M. C. (2007). Model calibration and issues related to validation, sensitivity analysis, post-audit, uncertainty evaluation and assessment of prediction data needs. In Groundwater: Resource evaluation, augmentation, contamination, restoration, modeling and management (pp. 237-282). Springer.

U.S. Geological Survey. (2024). MODFLOW 6 - Description of input and output (version 6.6.0). U.S. Geological Survey.

U.S. Geological Survey. (n.d.). Effective groundwater model calibration: With analysis of data, sensitivities, predictions, and uncertainty. Retrieved March 20, 2026, from https://www.usgs.gov/publications/effective-groundwater-model-calibration-analysis-data-sensitivities-predictions-and uncertainty.

U.S. Geological Survey. (n.d.). Guidelines 13 and 14 - Prediction uncertainty. Retrieved March 20, 2026, from https://www.usgs.gov/publications/guidelines-13-and-14-prediction-uncertainty

Zheng, C. (1990). MT3D, a modular three-dimensional transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems. S.S. Papadopulos & Associates.

Zheng, C., & Wang, P. P. (1999). MT3DMS: A modular three-dimensional multispecies transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems; documentation and user's guide. U.S. Army Engineer Research and Development Center.

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Appendix A. Equation Glossary and Symbol Definitions

This appendix consolidates the principal symbols used throughout the white paper. Symbols may be reused in different sub-contexts; where a context-specific meaning exists, the section-level equation definition governs.

- **a(k) -** random coefficient vector used in null-space Monte Carlo realization k
- **αL -** longitudinal dispersivity [L]
- **αT -** transverse dispersivity [L]
- **αex -** mobile-immobile mass-exchange coefficient [1/T]
- **b -** saturated thickness [L]
- **C -** aqueous contaminant concentration [M/L^3]
- **Cb -** boundary conductance [1/T]
- **Cp -** parent or precursor concentration [M/L^3]
- **Cim -** immobile-domain concentration [M/L^3]
- **Cs -** concentration of source or sink water [M/L^3]
- **Cp matrix -** parameter covariance matrix
- **D -** hydrodynamic-dispersion tensor [L^2/T]
- **Dm -** molecular diffusion coefficient in water [L^2/T]
- **ei -** residual for observation i
- **EEi -** Morris elementary effect
- **f(p) -** prior parameter distribution
- **f(p|y^{obs}) -** posterior parameter distribution
- **gp -** gradient of prediction Z with respect to parameters
- **h -** hydraulic head [L]
- **hB -** specified boundary head [L]
- **hR -** reference head for a head-dependent boundary [L]
- **I -** identity matrix
- **J -** Jacobian or sensitivity matrix
- **K -** hydraulic-conductivity tensor [L/T]
- **Kd -** linear sorption distribution coefficient [L^3/M]
- **Kf -** Freundlich sorption coefficient
- **L(p) -** likelihood or relative plausibility of parameter set p
- **m -** number of estimated parameters or withheld observations, depending on context
- **n -** number of observations
- **N -** number of Monte Carlo realizations or Freundlich exponent, depending on context
- **Pe -** cell Peclet number
- **p -** parameter vector
- **p* -** calibrated or optimal parameter vector
- **q -** Darcy flux vector [L/T]
- **qB -** specified boundary flux [L/T]
- **qs -** volumetric fluid source/sink term [1/T]

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Qm - mass source/sink term [M/L³/T]
R - retardation factor or reaction term, depending on context
RMSE - root mean square error
S - sorbed concentration [M/M]
Si - Sobol first-order sensitivity index
Ss - specific storage [1/L]
Sy - specific yield [-]
STi - Sobol total-effect index
t - time [T]
v - average linear groundwater velocity [L/T]
Var(Z) - variance of prediction Z
Vn - null-space basis matrix
W - source/sink term in the flow equation [1/T]
wi - observation weight
x, y, z - Cartesian coordinates [L]
Y - model output or prediction
yi_{obs} - observed value
yi_{sim} - simulated value
Z - selected prediction metric
θ - effective porosity or fluid content [-]
λ - first-order decay coefficient [1/T]
λs - first-order decay coefficient for sorbed mass [1/T]
λw - first-order aqueous decay coefficient [1/T]
μ - regularization weighting factor
ρ - fluid density [M/L³]
ρb - bulk density [M/L³]
σi^2 - observation-error variance
σpj - prior standard deviation for parameter j
σZ - prediction standard deviation
τ - tortuosity factor [-]
Φ - objective function

Appendix B. Supplementary Analytical and Numerical Equations Often Used in Groundwater Practice

The following equations are frequently used to bound parameter values, interpret field tests, or cross-check numerical-model behavior. They are not replacements for 3-D numerical modeling, but they remain valuable as sanity checks and calibration anchors.

Equation B-1. Theis confined-aquifer solution.

$$s(r,t) = \frac{Q}{4\pi T} W(u)$$

Where:

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s = drawdown [L]

r = radial distance from pumping well [L]

Q = pumping rate [L³/T]

T = transmissivity [L²/T]

W(u) = well function [-]

Equation B-2. Theis dimensionless time parameter.

$$u = \frac{r^2 S}{4Tt}$$

Where:

S = storativity [-]

Equation B-3. Cooper-Jacob late-time approximation.

$$s = \frac{2.3Q}{4\pi T}\log_{10}\left(\frac{2.25Tt}{r^2 S}\right)$$

Equation B-4. Hydraulic conductivity from transmissivity.

$$K = \frac{T}{b}$$

Where:

b = aquifer thickness [L]

Equation B-5. One-dimensional Darcy discharge.

$$q = -K\frac{dh}{dl}$$

Where:

i = hydraulic gradient [-]

A = cross-sectional area [L²]

Equation B-6. Simple advective travel time.

$$t_{adv} = \frac{n_e L}{Ki}$$

Where:

tb = travel time [T]

L = flow-path length [L]

Equation B-7. Contaminant mass flux through a control plane.

$$J = qC$$

Where:

M = mass discharge [M/T]

A = control-plane area [L²]

Equation B-8. Cumulative mass discharged across a plane.

$$M_{cum}(t) = \int_0^t J(\tau) A \, d\tau$$

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Where:

M_{cum} = cumulative discharged mass [M]

Equation B-9. River leakage term used in many finite-difference models.

$$Q_{riv} = C_{riv}(h_{riv} - h_{cell})$$

Where:

C_{riv} = riverbed conductance [L²/T]

h_{stage} = river stage [L]

h_{cell} = groundwater head in the adjacent model cell [L]

Equation B-10. General-head-boundary leakage term.

$$Q_{ghb} = C_{ghb}(h_b - h_{cell})$$

Where:

C_{ghb} = boundary conductance [L²/T]

h_{ghb} = external boundary head [L]

Equation B-11. Drain boundary flux.

$$Q_{drn} = \begin{cases} C_d(h_{cell} - h_d), & h_{cell} > h_d \\ 0, & h_{cell} \le h_d \end{cases}$$

Where:

Cdrn = drain conductance [L²/T]

hdrn = drain elevation [L]

Equation B-12. Conceptual evapotranspiration sink relation.

$$ET = ET_{max}\left(\frac{h - h_{ext}}{h_{surf} - h_{ext}}\right)$$

Where:

ET = evapotranspiration rate [L/T]

ETmax = maximum ET rate [L/T]

hET = extinction-surface elevation [L]

hext = extinction depth limit [L]

These relationships are often useful for scoping transmissivity, storativity, travel time, capture, or boundary conductance before the full 3-D model is finalized. A model that contradicts these first-order checks may still be correct, but it deserves closer scrutiny.

Appendix C. Validation, Post-Audit, and Data-Worth Equations

Formal validation of groundwater models is limited, but predictive corroboration can be strengthened using withheld data, post-audits, and data-worth analysis. The following metrics are commonly useful in technical review.

Equation C-1. Prediction error sum of squares using leave-one-out or analogous holdout tests.

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$$PRESS = \sum_{i=1}^{n} \left(y_i^{obs} - \hat{y}_{(-i),i}\right)^2$$

Where:

yi,-i = prediction for observation i from a calibration excluding i

Equation C-2. Akaike information criterion.

$$AIC = n\ln\left(\frac{RSS}{n}\right) + 2k$$

Where:

RSS = residual sum of squares

k = number of estimated parameters

Equation C-3. Bayesian information criterion.

$$BIC = n\ln\left(\frac{RSS}{n}\right) + k\ln n$$

Equation C-4. Conceptual data-worth metric for candidate new datum j.

$$DW_j = \frac{\sigma_Z^2 - \sigma_{Z|j}^2}{\sigma_Z^2}$$

Where:

DWj = data worth associated with datum j

Varbefore = prediction variance before collecting datum j

Varafter,j = prediction variance after collecting datum j

Equation C-5. Standardized predictive residual for a new or withheld datum.

$$r_{pred,j} = \frac{y_j^{obs} - y_j^{pred}}{\sigma_{pred,j}}$$

Where:

$\sigma_{pred,new}$ = prediction standard deviation for the new datum

These metrics should not be used mechanically. A lower AIC or BIC does not automatically make one conceptual model correct, and a large apparent data-worth estimate is only meaningful if the proposed measurement is actually feasible and decision-relevant.

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