Deliverables with GEO-FLUXES

A Reproducible Modeling Framework for Subsurface Flow, Transport, and Reactive Processes

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Overview

GEO-FLUXES deliverables are structured to scale with **data availability, project maturity, and decision needs**. Each deliverable set produces **fully traceable, reproducible modeling artifacts** designed to support technical review, risk assessment, and stakeholder communication.

All deliverables are generated through **deterministic, version-controlled workflows** integrating physics-based simulators (e.g., PFLOTRAN, FEHM, MODFLOW, VS2DI, VS2DTI) with automated preprocessing, postprocessing, QA/QC, and reporting layers. Every figure, table, and conclusion is explicitly traceable to its underlying assumptions, inputs, and solver configurations.

Core Deliverable Principles

All GEO-FLUXES deliverables include:

- Explicitly documented modeling assumptions and limitations
- Solver configurations and numerical controls preserved for reruns
- QA/QC checks applied consistently across scenarios
- Version-controlled inputs, scripts, and outputs
- Reproducible directory structures linking inputs to results

This ensures results are **defensible, auditable, and review-ready**.

Deliverable Sets by Project Phase

Deliverable Set A — Rapid Screening and Feasibility Assessment (2–4 Weeks)

Objective: Provide a defensible first-pass evaluation to inform go/no-go decisions and prioritize data collection.

Deliverables

- Screening-scale models sized to available information, capturing:
  - Injectivity and pressure response
  - First-order plume or influence-zone behavior
  - Dominant flow and transport controls
- Targeted sensitivity analysis identifying parameters that most strongly influence outcomes (e.g., permeability, relative permeability, salinity, temperature)
- Explicit articulation of:

    - Assumptions
    - Known limitations
    - Critical data gaps
- Concise, decision-focused PDF report summarizing:
    - Modeling approach
    - Key results and sensitivities
    - Recommended next steps and risk-reduction priorities

Deliverable Set B — Site Concept Model and Operational Scenarios (6–12 Weeks)

Objective: Develop a technically consistent site-scale model suitable for engineering evaluation and scenario comparison.

Deliverables

- Site-scale conceptual and numerical model including:
    - Domain definition, stratigraphy, and heterogeneity representation
    - Initial and boundary conditions consistent with available site data
- One or more well configurations and operational schedules with explicit constraint checks (e.g., pressure limits, rate limits, fracture thresholds)
- Scenario comparisons evaluating alternative operational strategies
- Decision-ready outputs including:
    - Pressure envelopes and spatial diagnostics
    - Plume evolution and containment indicators
    - Flow and transport metrics relevant to operations
- Fully reproducible model package containing:
    - Input files and run instructions
    - Standardized plots and summary tables
    - QA/QC summaries and run logs

Deliverable Set C — Reactive Transport, Mineralization, and Long-Term Performance (6–12 Weeks)

Objective: Quantify geochemical processes and long-term system behavior where permanence, transformation, and interaction are critical.

Deliverables

- Chemistry and reaction configuration including:
    - Relevant aqueous species, minerals, and reaction pathways
    - Reaction rate formulations and thermodynamic database selection
- Coupled flow–transport–reaction simulations
- Time-resolved partitioning of fluids and solutes among:
    - Mobile or free-phase
    - Dissolved phase

- Mineralized or immobilized fractions
- Permanence and transformation key performance indicators (KPIs) suitable for:
  - Technical narratives
  - Risk and uncertainty discussions
- Explicit documentation of:
  - Geochemical assumptions
  - Parameter uncertainty
  - Modeling limits and applicability

Deliverable Set D — MRV-Ready, Audit-Grade Modeling Package (Ongoing)

Objective: Provide a defensible, updateable modeling framework suitable for monitoring, reporting, and verification (MRV) contexts.

Deliverables

- Standardized QA/QC checklist applied to each model update
- Versioned scenario library enabling consistent comparison over time
- Traceable run logs linking:
  - Inputs
  - Solver settings
  - Outputs and derived metrics
- Monitoring and data-value assessment identifying:
  - Measurements that most constrain pressure, plume, and transport behavior
  - Data priorities for reducing uncertainty
- Consistent reporting format suitable for:
  - Internal governance
  - External technical review
  - Regulatory-style documentation

Organization and Traceability

All GEO-FLUXES deliverables follow a consistent, reproducible directory structure, typically including:

- `/inputs/` — conceptual models, parameter files, and assumptions
- `/models/` — solver-specific input decks
- `/runs/` — execution logs and metadata
- `/tables/` — parsed and standardized CSV outputs
- `/figures/` — publication-quality plots
- `/reports/` — Markdown and PDF technical reports

This structure preserves a transparent artifact chain from raw assumptions to final deliverables.

Intended Use

GEO-FLUXES deliverables are intended to support:

- Interpretation and comparison of subsurface scenarios
- Engineering and risk-informed decision-making
- Communication with technical reviewers and stakeholders

They are **not intended as standalone predictive forecasts**, but as **defensible, traceable scientific products** that explicitly communicate uncertainty and limitations.

Why This Is Valuable

GEO-FLUXES transforms complex subsurface problems into **transparent, testable, and repeatable modeling workflows**. By integrating multiple physics-based simulators within a single, coherent framework, GEO-FLUXES:

- Reduces technical and decision risk
- Improves consistency across modeling approaches and spatial scales
- Enables rigorous sensitivity, calibration, and uncertainty analysis
- Produces audit-ready artifacts that withstand technical scrutiny

The result is **faster insight, clearer uncertainty communication, and stronger technical justification** for decisions related to subsurface energy systems, environmental management, and storage applications.
