GEO-FLUXES

Multiphase Flow and Transport Modeling for Subsurface Energy and Storage Systems

Executive Summary

GEO-FLUXES is a comprehensive, Python-driven computational framework for subsurface flow, transport, and coupled process modeling across energy, environmental, and storage applications. The platform integrates multiple, well-established numerical simulators—including **PFLOTRAN**, **FEHM**, **MODFLOW**, **VS2DI**, and **VS2DTI**—within a unified, transparent, and reproducible workflow.

GEO-FLUXES is designed to support the **full modeling lifecycle**, from conceptual model development and scenario design to simulation execution, postprocessing, parameter estimation, uncertainty analysis, and decision-ready reporting. By combining solver-appropriate physics with a consistent Python orchestration layer, the framework preserves the numerical strengths of each engine while eliminating fragmentation in setup, analysis, QA/QC, and documentation.

The platform delivers **traceable simulation packages**, operational scenarios with explicit physical and engineering constraints, and **decision-ready outputs** suitable for technical review, regulatory-style documentation, and stakeholder communication. Emphasis is placed on physical realism, transparent assumptions, reproducibility, and defensible uncertainty framing, enabling robust evaluation of **groundwater flow**, **multiphase and gas–liquid systems**, **reactive transport**, **near-field and variably saturated processes**, **microfluidic and pore-scale behavior**, and **long-term system performance** across a wide range of subsurface applications.

Capabilities

GEO-FLUXES provides an integrated, multi-scale modeling capability spanning laboratory, field, and regional domains. Each capability leverages the most appropriate numerical engines while maintaining a consistent workflow for scenario definition, execution control, postprocessing, parameter estimation, QA/QC, and reporting.

Groundwater Flow and Solute Transport

GEO-FLUXES supports saturated groundwater flow and solute transport modeling for environmental, energy, and infrastructure applications.

What We Can Do

- Regional- and site-scale groundwater flow modeling
- Hydraulic head and pressure evolution under natural and engineered stresses
- Conservative and reactive solute transport
- Recharge, boundary-condition, and property sensitivity analysis

Primary engines

- MODFLOW and MODFLOW-family tools

Supporting engines

- PFLOTRAN (density-dependent flow and coupled transport)
- FEHM (flow with thermal coupling)

Multiphase Flow (CO_2, H_2, Gas–Water Systems)

GEO-FLUXES supports multiphase flow and gas–liquid interaction modeling across reservoir-scale, near-field, and transition-zone regimes.

What We Can Do

- Gas injection scenarios with pressure buildup and plume migration
- Buoyancy-driven flow, containment, and trapping behavior
- Salinity- and temperature-dependent effects
- Coupled saturated–unsaturated transitions near wells and boundaries

Primary engines

- PFLOTRAN — multiphase gas–water flow and compositional effects
- FEHM — multiphase and thermal–hydrologic systems

Supporting engines

- MODFLOW-family (density-aware formulations)
- VS2DI / VS2DTI for near-field and partially saturated zones

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Wells, Operations, and Engineering Constraints

GEO-FLUXES represents coupled wells and operational controls under realistic engineering and regulatory constraints.

What We Can Do

- Injection and production scheduling (CO_2, H_2, brine, water)
- Pressure, rate, and fracture-gradient constraint enforcement
- Well interference analysis and operational trade studies
- Field-level performance metrics and diagnostics

Primary engines

- PFLOTRAN
- FEHM

Supporting workflows

- MODFLOW well packages
- Python-based operational logic for scheduling and constraint handling

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Reactive Transport and Geochemical Processes

GEO-FLUXES incorporates reactive transport where geochemistry governs system evolution and long-term behavior.

What We Can Do

- Coupled flow, transport, and geochemical reaction modeling
- Mineral dissolution and precipitation
- Gas partitioning and phase exchange
- Time-dependent mass balance and reaction-path analysis
- Permanence, storage, and transformation metrics with explicit assumptions

Primary engines

- PFLOTRAN

Supporting workflows

- Python-based reaction bookkeeping, diagnostics, and reporting

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Variably Saturated Flow and Near-Field Processes

GEO-FLUXES supports vadose-zone and near-surface modeling where capillary effects and partial saturation dominate.

What We Can Do

- Variably saturated flow and transport simulations
- Infiltration, leakage, and near-field process representation
- Coupling of vadose-zone and deeper saturated or multiphase systems

Primary engines

- VS2DI
- VS2DTI

Microfluidic and Pore-Scale Simulations

GEO-FLUXES supports microfluidic, pore-scale, and laboratory-scale simulations for process understanding, benchmarking, and scale-bridging.

What We Can Do

- Flow and transport in microfluidic and lab-on-chip geometries

- Geometry-controlled experiments and synthetic pore networks
- Upscaling insights to inform continuum-scale models

Primary engines

- PFLOTRAN (micro-domain configurations)
- FEHM (small-scale domains)

Supporting workflows

- Python-based geometry generation, meshing, and analysis

Parameter Estimation, Inverse Modeling, and Uncertainty Analysis

GEO-FLUXES provides parameter estimation and inverse modeling capabilities across all supported simulators.

What We Can Do

- Calibration of hydraulic, transport, thermal, and reactive parameters
- Gradient-free, ensemble-based, and sampling-driven inverse workflows
- Sensitivity analysis, identifiability assessment, and uncertainty propagation
- Cross-solver parameter comparison and risk framing

Supported engines

- PFLOTRAN
- FEHM
- MODFLOW
- VS2DI
- VS2DTI

Integration layer

- Python-based optimization, sampling, and diagnostic tools

Postprocessing, KPIs, and Reporting

GEO-FLUXES converts raw simulator outputs into consistent, decision-ready products.

What We Can Do

- Automated plots for pressure, flow, plume extent, and transport metrics
- Mass balance, storage partitioning, and diagnostic KPIs
- Cross-solver comparison and standardized reporting
- Outputs suitable for technical, regulatory, and stakeholder review

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Reproducibility, QA/QC, and Audit Readiness

GEO-FLUXES is designed to produce defensible, auditable results.

What We Can Do

- Fully reproducible run packages with complete provenance
- Solver-agnostic QA/QC (mass balance, stability, convergence checks)
- Versioning, change tracking, and assumptions registers
- Transparent linkage from inputs to final deliverables

Why This Matters for Clients

GEO-FLUXES reduces technical risk by transforming complex subsurface problems into **transparent, testable, and repeatable modeling workflows**. By supporting groundwater flow, multiphase systems, reactive transport, parameter estimation, and pore-scale processes within a single coherent platform, GEO-FLUXES enables faster insight, clearer uncertainty communication, and stronger technical justification for decisions related to energy systems, environmental management, and subsurface storage.