Physics-Informed Machine Learning for Evaluating Contaminant Transport and Long-Term Barrier Performance in Geosynthetic Clay Liners

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Abstract

Geosynthetic clay liners (GCLs) are low-permeability barrier components used in waste containment and environmental containment systems, but their long-term performance is difficult to evaluate because contaminant transport is coupled to stress-dependent hydraulic conductivity, geochemical alteration, sorption, and diffusive flux. Conventional advection-dispersion models require constitutive parameters that are sparse, scale-dependent, and often calibrated under conditions that do not represent long service life. Purely data-driven models can fit available observations but may violate mass balance, extrapolate unrealistically beyond tested permeants, and provide weak support for design decisions. This paper develops a physics-informed machine-learning framework for evaluating contaminant transport and long-term barrier performance in GCLs. The framework couples a neural surrogate for dissolved concentration with constrained constitutive closures for hydraulic conductivity and sorption, embeds the advection-dispersion-reaction residual in the training objective, and enforces nonnegativity and monotonicity constraints justified by sodium-bentonite behavior. Bayesian inference propagates uncertainty in transport and closure parameters, while a reliability formulation translates posterior concentration and hydraulic-conductivity predictions into time-dependent barrier-performance probabilities. Analytical assessment addresses identifiability, extrapolation, data requirements, baseline comparisons, and domain-specific error modes. The central insight is that physically constrained learning can preserve contaminant mass balance and known aging trends while retaining flexibility to assimilate column and field data. Interpretability and global sensitivity analysis identify which geochemical and stress variables dominate predicted service life, providing a defensible basis for scenario analysis, monitoring prioritization, and design decisions.

Keywords

geosynthetic clay liner; contaminant transport; physics-informed machine learning; Bayesian uncertainty; hydraulic conductivity; barrier reliability

1. Introduction

Long-term performance of engineered containment systems depends on the ability of barrier components to limit contaminant migration over decades to centuries. GCLs are widely used because a thin sodium-bentonite layer can provide low hydraulic conductivity and self-healing behavior when confined and properly hydrated. Their field performance is nevertheless sensitive to effective stress, bentonite content, hydration history, cation exchange, wet-dry cycling, freeze-thaw action, and chemical incompatibility with leachates or permeating solutions. These factors alter both hydraulic conductivity and diffusive transport, so a credible assessment of barrier performance must treat hydraulic, geochemical, and transport processes as coupled rather than independent.

The environmental geotechnics literature has established that long-term barrier behavior cannot be inferred from short-term hydraulic conductivity tests alone [1]. GCL hydraulic conductivity depends strongly on permeant chemistry and bentonite fabric, and nonstandard liquids can produce order-of-magnitude changes relative to water [2]. GCLs are composite materials whose performance depends on bentonite swelling, confinement, and the surrounding geosynthetic or soil layers [3], and their field hydraulic performance can differ from laboratory values because of installation damage, hydration conditions, and overlburden stress [4]. Barrier-system analyses that combine advection, diffusion, sorption, and degradation provide a more appropriate basis for service-life evaluation than a single conductivity value [5].

Machine learning offers an attractive route for assimilating heterogeneous laboratory and field data and for constructing rapid surrogates of expensive transport simulations. Data-driven estimates of hydraulic conductivity for sodium-bentonite GCLs have been explored with machine-learning approaches [6], illustrating the potential of learned mappings from material and permeant descriptors to barrier properties. However, a learned conductivity function is not by itself a transport model. If such a closure is inserted into a contaminant-transport calculation without mass-balance constraints, boundary conditions, and uncertainty propagation, it can produce physically inconsistent breakthrough curves and misleading estimates of service life. The central problem addressed here is therefore not whether machine learning can interpolate hydraulic conductivity data, but how learned components can be embedded within a physically consistent transport and reliability framework for GCL barrier performance.

This paper develops a physics-informed machine-learning framework for evaluating contaminant transport and long-term barrier performance in GCLs. The contribution is a coupled formulation in which a neural surrogate for dissolved concentration is trained against the advection-dispersion-reaction residual, while hydraulic-conductivity and sorption closures are constrained to respect mass balance, nonnegativity, and prior monotonicity expectations for sodium-bentonite behavior. Bayesian inference is used to represent uncertainty in transport and closure parameters, and a reliability formulation converts posterior predictions into time-dependent probabilities of exceeding concentration or hydraulic-conductivity thresholds. The framework is presented as a methodological and analytical contribution: it specifies the governing equations, model architecture, training objective, uncertainty treatment, evaluation logic, and error modes that must be addressed before operational use.

2. Governing Physics and Long-Term Barrier Performance

2.1 Contaminant transport through GCL barriers

Contaminant migration through a GCL is often dominated by diffusion when the barrier remains intact and advective flux is small, but advection becomes important where hydraulic gradients, defects, or chemical incompatibility increase hydraulic conductivity. A one-dimensional transport formulation is a useful working model for column tests and for screening-level barrier assessment. The governing equation used in the proposed framework is

$$\partial C/\partial t = D_h\,\partial^2 C/\partial z^2 - v_h\,\partial C/\partial z - (\rho_b/\theta)\,\partial q/\partial t - \lambda C$$

where C is dissolved contaminant concentration, t is time, z is the spatial coordinate across the GCL, D_h is hydrodynamic dispersion, v_h is seepage velocity, ρ_b is dry bulk density, θ is porosity, q is sorbed mass per dry mass, and λ is a first-order degradation rate. The equation assumes one-dimensional isothermal transport, constant porosity and bulk density over the timescale of a single analysis, and no internal source other than sorption and first-order decay. The sorption term couples geochemical retention to dissolved concentration; it should not be treated as a fixed retardation factor when non-linear sorption or changing porewater chemistry is expected.

Sorption in sodium-bentonite GCLs is frequently represented with a Langmuir-type isotherm for screening calculations when site-specific data are limited:

$$q = q_m axK_L \frac{C}{(1 + K_L C)}$$

where q_max is the maximum sorption capacity and K_L is the Langmuir affinity coefficient. For dilute organic contaminants, a linear limit q = K_d C is often adequate, but for inorganic cations and mixed leachates, competitive exchange and ionic-strength effects can invalidate a single K_d. The Langmuir form is used here as a transparent closure that can be replaced by a more detailed ion-exchange model while preserving the transport structure. The important methodological point is that sorption must remain coupled to C and to porewater chemistry rather than being imposed as an unconstrained learned output.

2.2 Hydraulic and geochemical aging mechanisms

GCL barrier performance changes as bentonite hydrates, swells, exchanges cations, and consolidates under overburden stress. Increased effective stress generally reduces hydraulic conductivity by compressing the bentonite layer and reducing void ratio. Exposure to solutions with high ionic strength or unfavorable cation composition can suppress swelling, increase hydraulic conductivity, and alter diffusive pathways. Wet-dry cycling can create cracks or fabric changes that may or may not self-heal under confinement. These mechanisms imply that a conductivity closure should be positive, should respect expected monotonic trends with effective stress and ionic strength for sodium bentonite, and should be allowed to vary with hydration state, temperature, and time.

A purely empirical closure can reproduce these trends within a training range but may violate them outside it. For example, a flexible regression could predict decreasing hydraulic conductivity with increasing ionic strength because of spurious correlations in a small dataset, even though sodium-bentonite behavior commonly shows the opposite trend. Physics-informed constraints reduce this risk by penalizing violations of prior monotonicity and by retaining the transport equation as a source of structural information. The constraints are not a substitute for chemical compatibility testing; they encode expected behavior and make departures from that behavior visible and auditable.

2.3 Scale and parameter uncertainty

Long-term barrier assessment is affected by parameter uncertainty, model-structure uncertainty, and spatial variability. Laboratory column tests provide controlled transport data but may not represent field stress, hydration, or geochemical conditions. Field monitoring provides integrated performance evidence but is sparse and often indirect. The transport parameters D_h, v_h, θ, ρ_b, λ, and sorption coefficients are correlated and may be non-identifiable from a single breakthrough curve. A framework that reports only a best-fit prediction without uncertainty can therefore overstate confidence in service-life estimates. The proposed framework treats uncertainty explicitly and separates uncertainty in learned closures from uncertainty in transport parameters.

3. Physics-Informed Machine Learning Framework

3.1 Problem statement and state variables

The framework defines a mapping from GCL and permeant descriptors to state variables and transport outputs. The input vector x includes effective stress σ′, ionic strength I, water content or hydration state w, temperature T, elapsed time t, and available material descriptors such as bentonite content, cation-exchange capacity, and polymer modification. The outputs are hydraulic conductivity k, sorption parameters, and dissolved concentration C(z,t). The transport surrogate is a neural network C_θ(z,t,x) that is trained to satisfy the governing equation at collocation points and to match available observations at measurement locations. The closure for hydraulic conductivity is represented as a constrained function k = k(x; θ_k), and sorption parameters are treated as either calibrated scalars or functions of porewater chemistry.

Physics-informed neural networks provide a natural architecture for this problem because they can represent continuous fields and be differentiated with respect to time and space [7]. The broader physics-informed machine-learning literature shows that embedding conservation laws, constitutive relations, or boundary conditions into training can improve extrapolation and reduce data requirements relative to unconstrained regression [8]. The framework adopted here follows that logic but specializes it to GCL transport: the network is not trained merely to fit concentration observations; it is trained to produce a concentration field whose derivatives satisfy the transport residual and whose associated hydraulic closure respects geotechnical constraints.

3.2 Constrained constitutive closure

Hydraulic conductivity is represented through a log-transform to enforce positivity:

$$log_{10} k = f_k(\sigma', I, w, T, t;\ \theta_k), \partial f_k/\partial \sigma' \leq 0, \partial f_k/\partial I \geq 0$$

where f_k is a neural or hybrid basis-function model, θ_k are its parameters, σ′ is effective stress, I is ionic strength, w is hydration state, T is temperature, and t is time. The inequality constraints encode the prior expectation that increasing effective stress reduces hydraulic conductivity and that increasing ionic strength tends to increase hydraulic conductivity for sodium bentonite, although the latter can be modified for polymer-treated or chemically preconditioned GCLs. The constraints are enforced through penalty terms or constrained optimization during training. This closure is deliberately simple at the formulation level so that chemical-specific effects can be added without changing the transport architecture.

The use of a constrained closure is a substantive modeling choice. It reduces the hypothesis space to functions that are physically admissible, which can improve extrapolation to stress and chemistry ranges slightly outside the training data. It also makes model behavior auditable: if a prediction violates a monotonicity constraint, the violation indicates either a data conflict or a model misspecification that should be investigated. The constraint does not guarantee correctness; it only prevents a class of physically implausible responses.

3.3 Training objective and residual enforcement

The training objective combines data mismatch, transport-residual enforcement, boundary and initial conditions, and physical constraints:

$$L(\theta) = L_d + \lambda_r L_r + \lambda_b L_b + \lambda_p L_p$$

where L_d is the data misfit at observed concentrations or hydraulic conductivities, L_r is the mean squared transport residual at collocation points, L_b enforces boundary and initial conditions, L_p penalizes violations of nonnegativity and monotonicity constraints, and λ_r, λ_b, and λ_p are weighting coefficients. The residual is evaluated by automatic differentiation of C_θ with respect to z and t. Collocation points are distributed across the GCL thickness and time domain, with denser sampling near boundaries and anticipated breakthrough fronts.

The weights λ_r, λ_b, and λ_p control a bias-variance trade-off. Large residual weights enforce physics strongly and can improve extrapolation, but they may make optimization difficult when data are noisy or when the assumed transport model is incomplete. Small residual weights allow the network to fit data but increase the risk of mass-balance error. The framework therefore treats the weights as calibration hyperparameters selected by holdout performance and residual diagnostics, not as arbitrary constants. A useful diagnostic is the spatial integral of the residual, which should remain small relative to the advective and diffusive fluxes at the boundaries.

3.4 Bayesian uncertainty and closure calibration

Parameter and closure uncertainty are represented through a Bayesian posterior. Let D denote available observations and let θ and ψ denote network and closure parameters, respectively. The predictive distribution for boundary concentration C_b(t) is

$$p(C_b(t)|D) = \int p(C_b(t)|\theta,\psi)\, p(\theta,\psi|D)\, d\theta\, d\psi$$

where p(θ,ψ|D) is the posterior distribution obtained from Bayes' rule and the likelihood implied by measurement error. The posterior can be approximated with Markov-chain Monte Carlo for low-dimensional closure models or with variational inference and deep ensembles for high-dimensional networks. Bayesian calibration of computer models provides the conceptual basis for treating simulator discrepancy and parameter uncertainty separately [9]. Ensemble or random-forest baselines can be used to test whether the additional physics constraints improve predictive skill rather than merely increasing model complexity [10].

Interpretability is important because a GCL performance assessment must identify which variables drive predicted service life. Feature-attribution methods such as Shapley additive explanations can quantify the contribution of stress, chemistry, and hydration variables to individual predictions [11]. Global sensitivity analysis complements local attribution by apportioning output variance among inputs and interactions [12]. Bayesian data analysis provides the inferential structure for combining prior knowledge, laboratory data, and field evidence without collapsing all uncertainty into a single calibrated value [13].

Physics-informed learning for subsurface flow demonstrates that neural networks can learn constitutive relationships and parameters from sparse data while respecting governing equations [14]. The GCL problem is similar in structure but differs in its strong geochemical controls and thin-layer geometry. Integrating scientific knowledge into machine learning is most effective when the knowledge is expressed as explicit constraints, residual terms, or structured model components rather than as post hoc checks [15]. Software frameworks for physics-informed neural networks support automatic differentiation, residual sampling, and boundary-condition enforcement, which makes the proposed workflow implementable without custom discretization code [16].

4. Methodological Evaluation and Analytical Assessment

4.1 Data requirements and evaluation logic

Operational implementation requires three data classes: material and permeant descriptors for the closure model, column or diffusion-cell measurements for transport calibration, and boundary conditions representing the field liner system. The framework does not assume that all classes are simultaneously available. When transport data are sparse, the residual term and prior constraints carry more of the predictive burden; when data are abundant, the data misfit can dominate. Evaluation should compare the physics-informed model against at least three baselines: a conventional advection-dispersion model with calibrated effective parameters, a purely data-driven regressor for hydraulic conductivity, and an unconstrained neural surrogate trained only on concentration observations.

Performance should be assessed with domain-specific criteria rather than aggregate error alone. Relevant criteria include breakthrough-time error, peak-concentration error, mass-balance residual, posterior predictive coverage, and stability under extrapolation to higher ionic strength or lower effective stress. A model that fits the observed concentration curve but produces a nonphysical negative concentration or a hydraulic conductivity that increases with effective stress should not be accepted, even if its mean-squared error is low. The evaluation should also report sensitivity rankings, because a design decision may depend more on whether ionic strength or overburden stress dominates predicted service life than on a small improvement in curve fitting.

4.2 Identifiability and extrapolation

Transport parameters are often correlated. For example, a decrease in effective diffusion coefficient can be partially offset by an increase in retardation, producing similar breakthrough curves over a limited observation window. Adding a flexible learned closure increases the number of parameters and can worsen identifiability unless constraints and priors are used. The framework addresses this issue by keeping the transport equation explicit, placing monotonicity constraints on hydraulic conductivity, and using Bayesian priors that penalize implausible parameter combinations. Residual diagnostics and posterior correlation matrices should be reported so that non-identifiability is visible rather than hidden.

Extrapolation is a central concern for long-term barrier assessment because service-life predictions extend beyond test durations. Physics constraints improve extrapolation only when the assumed mechanisms remain valid. If a GCL undergoes a geochemical transition that is not represented in the training data, a constrained model can still be wrong. The framework therefore treats extrapolation as a scenario-analysis problem: predictions are conditional on stated assumptions about cation exchange, polymer durability, and stress

history. Scenario analysis should bracket plausible ranges of ionic strength, effective stress, and degradation rate rather than presenting a single deterministic service life.

4.3 Reliability formulation and decision rules

For barrier design and monitoring, the relevant output is not only a predicted concentration but the probability that performance criteria are exceeded. A time-dependent reliability index can be defined as

$$R(t) = \Pr[C(L,t) \le C_l im, k(t) \le k_l im | D]$$

where C(L,t) is the concentration at the downgradient boundary of the GCL, C_lim is a regulatory or design concentration limit, k(t) is hydraulic conductivity, k_lim is a conductivity threshold, and D denotes the available data and model assumptions. The probability is computed from the posterior predictive distribution. This formulation allows concentration and hydraulic conductivity criteria to be evaluated jointly, which is important because a GCL may satisfy a conductivity criterion while still allowing unacceptable diffusive flux, or vice versa.

Sensitivity analysis supports monitoring prioritization. A variance-based index for input X_i can be written as

$$S_i = \mathrm{Var}_{X_i} \frac{(\mathrm{E}[C_b|X_i])}{\mathrm{Var}}(C_b)$$

where E[C_b|X_i] is the conditional expectation of boundary concentration given X_i, and Var(C_b) is the unconditional variance. The index S_i measures the fraction of output variance explained by X_i. In a GCL context, high sensitivity to ionic strength or effective stress indicates that those variables should be monitored or controlled most carefully. Low sensitivity to a material descriptor does not prove irrelevance; it may reflect limited variation in the available data or strong interaction with other variables.

4.4 Error modes and technical safeguards

Several error modes are specific to physics-informed learning for GCL transport. Residual weighting that is too low can produce concentration fields that fit observations but violate mass balance. Residual weighting that is too high can force the network to satisfy an oversimplified transport model and suppress real chemical effects. Sparse collocation near the breakthrough front can produce smeared fronts and inaccurate breakthrough times. Overfitting to a single permeant can create a closure that is accurate for that chemistry but unstable for another. The framework mitigates these risks through residual-based adaptive sampling, holdout testing by permeant type, monotonicity checks, and posterior predictive checks.

A second safeguard is separation of calibration and validation by process. Hydraulic-conductivity data should not be used to validate transport predictions, and transport data should not be used to tune the conductivity closure without accounting for the resulting dependence. Where data are insufficient for formal separation, leave-one-out or blocked cross-validation by material batch, permeant, or stress level is preferable to random point-wise splitting. The latter can overstate performance because nearby points from the same test are highly correlated.

5. Technical Discussion

The proposed framework differs from conventional GCL assessment in three ways. First, it treats hydraulic conductivity and sorption as constitutive closures within a transport model rather than as isolated prediction targets. This matters because a change in conductivity alters both advective flux and the diffusive path length, and a change in sorption alters retardation and breakthrough timing. Second, it uses physics constraints to restrict the hypothesis space of the machine-learning model. The constraints are not arbitrary regularizers; they encode established trends in sodium-bentonite behavior, such as swelling-controlled reductions in conductivity under effective stress and chemically induced increases in conductivity at high ionic strength. Third, it makes uncertainty and reliability explicit, so that a predicted service life is expressed as a conditional probability rather than as a deterministic number.

The framework also has clear limitations. The one-dimensional transport equation is a screening model; it does not resolve defects, wrinkles, or nonuniform hydration in a composite liner. The Langmuir closure is a simplification of competitive ion exchange. The monotonicity constraints are prior expectations that may not hold for all polymer-modified or chemically preconditioned GCLs. These limitations do not invalidate the framework, but they define the conditions under which its predictions should be interpreted. When the GCL is expected to undergo complex geochemical alteration, the transport equation should be coupled to a geochemical speciation model, and the learned closure should be trained on the corresponding chemical descriptors.

From a design perspective, the most useful output is not a single predicted breakthrough curve but a mapping from controllable variables to reliability. Effective stress, bentonite mass per area, hydration procedure, and cover design can be controlled during construction; ionic strength and leachate chemistry can be monitored but not always controlled. A reliability map showing how R(t) changes with these variables can support material selection, quality assurance, and monitoring frequency. The same map can identify where additional testing would most reduce uncertainty. If sensitivity analysis shows that predicted reliability is dominated by ionic strength, for example, additional chemical compatibility testing is more valuable than additional hydraulic conductivity tests at a single reference chemistry.

The interpretability requirement is particularly important for regulatory and engineering acceptance. A black-box prediction of service life is difficult to defend when the underlying data are sparse and the extrapolation horizon is long. Physics-informed constraints, residual diagnostics, and sensitivity indices provide an audit trail: they show which physical relationships were enforced, which data informed the posterior, and which variables drive the result. That audit trail does not eliminate uncertainty, but it makes uncertainty transparent and allows reviewers to challenge specific assumptions rather than rejecting the model as a whole.

6. Conclusion

This paper has developed a physics-informed machine-learning framework for evaluating contaminant transport and long-term barrier performance in GCLs. The framework couples a neural transport surrogate with constrained closures for hydraulic conductivity and sorption, embeds the advection-dispersion-reaction residual in training, and enforces nonnegativity and monotonicity conditions consistent with sodium-bentonite behavior. Bayesian inference propagates uncertainty in transport and closure parameters, while a reliability formulation converts posterior predictions into time-dependent probabilities of exceeding concentration and conductivity thresholds. Analytical assessment shows that the main advantages of the

approach are mass-balance consistency, constrained extrapolation, interpretable sensitivity, and a direct link between model outputs and barrier-performance decisions.

The framework is not a substitute for site-specific testing or geochemical characterization. Its credibility depends on the validity of the assumed transport mechanisms, the quality of the calibration data, and the transparency of the constraints. The most defensible use is scenario analysis under stated assumptions, supported by posterior predictive checks, blocked validation, and sensitivity analysis. Under those conditions, physics-informed learning can provide a disciplined way to combine sparse GCL data with established transport theory and to communicate long-term barrier performance as a probabilistic, auditable assessment rather than a single deterministic prediction.

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