

Original Research

Climate Change Impacts on Pesticide Leaching in Agricultural Soils: A PEARL (Pesticide Emission Assessment at Regional and Local) Model Assessment for S-Metolachlor under CMIP6 (Coupled Model Intercomparison Project Phase 6) Scenarios

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Abstract

Climate change represents a significant risk to groundwater quality by altering the dynamics of pesticide transport in agricultural soils. This study assesses the influence of expected climate change using the PEARL (Pesticide Emission Assessment at Regional and Local scales) framework on S-metolachlor pesticide leaching. This analysis was based on agricultural loam soil, a historical baseline (1981-2010), and two future scenarios: SSP2-4.5 (medium-emission scenario) and SSP5-8.5 (high-emission scenario) from 2041 to 2070. Calibration with field-derived data ($DT_{50} = 18 \pm 4$ days, $K_{oc} = 200$ mL/g) and validation with groundwater observation data showed increased cumulative pesticide leaching by +60.5% (SSP2-4.5) and +110.7% (SSP5-8.5) compared to historical data. This indicates that the concentration might exceed the regulatory limits by a factor of 0.15-0.25 $\mu\text{g/L}$ (compared with the EU groundwater limit of 0.1 $\mu\text{g/L}$). Reduced sorption at higher temperatures, together with increased precipitation, synergistically enhanced pesticide transport. These findings indicate that current pesticide

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risk assessments may underestimate future groundwater contamination potential, necessitating climate-adaptive regulatory frameworks and management strategies to protect drinking water quality.

Keywords: pesticide leaching, climate change, groundwater contamination, PEARL model, regulatory threshold, drinking water quality, S-metolachlor

Introduction

Pesticide contamination of groundwater is a major environmental concern that continues to pose a threat to the health of the population in agricultural areas around the world [1, 2]. Groundwater is the major source of drinking water for 50% of the world's population and over 95% of the population in the countryside [3, 4]. The contamination of groundwater by pesticide residues has resulted in the enforcement of very strict regulations, such as the EU groundwater directive (0.1 µg/L detection limit for each pesticide individually) and the WHO guidelines (10 µg/L detection limit for each pesticide individually) [4, 5]. Decades after the establishment of regulatory controls, pesticide contamination data from groundwater remain widespread, with herbicides being most frequently detected [6]. S-metolachlor, a selective chloroacetanilide herbicide, is among the most widely applied agricultural pesticides globally, with extensive use in corn and soybean production systems [7]. Moderate persistence and mobility values (soil half-life of 15-25 days and Koc of 120-280 mL/g) rank it as a substance of emerging priority with respect to the protection of groundwater resources [8]. Numerous field studies have reported the occurrence of S-metolachlor in shallow groundwater across key agricultural belts, with detection frequencies between 35 and 52% in intensely agricultural areas [9]. Its widespread application, known fate characteristics, and importance as a regulated substance qualify it as a suitable model substance that can be used to evaluate the effects of climate change on its leachability.

Climate change is causing radical shifts in the hydrological and thermal cycles that regulate pesticide behavior in agricultural soils [10, 11]. Projected temperature increases of 1.5°C to 4.5°C by 2100, together with changes in precipitation, are predicted to affect the mechanisms controlling pesticide mobility in soils, including degradation, adsorption, and water flux [12]. Recent studies have demonstrated that climate-induced changes in soil moisture, temperature, and precipitation intensity can substantially alter pesticide leaching potential [13-18]. However, most current pesticide risk assessments rely on historical climate data and do not account for projected future conditions, potentially underestimating long-term groundwater contamination risks [19].

Mechanistic pesticide fate models are important tools for predictive risk assessment even under conditions of environmental change [20-23]. A widely used risk assessment framework is PEARL (Pesticide Emission Assessment at Regional and Local scales),

which has been well validated and employed as a risk assessment tool by various environmental authorities, including the European Food Safety Authority (EFSA), as well as country pesticide registration authorities [20-24]. PEARL combines basic processes of pesticide fate: degradation, sorption, convective-dispersive transport processes, along with climate-related calculations of water balance to simulate pesticide concentrations in soil and leachate [25]. When equipped with field-tested parameters, PEARL-based risk assessment models can be useful tools to predict pesticide behavior even under new climate scenarios [26].

This study aims to: (1) quantify the impact of projected climate change on S-metolachlor leaching in standard agricultural soil using a validated PEARL model framework; (2) assess future groundwater concentration projections against regulatory thresholds (WHO 10 µg/L and EU 0.1 µg/L); (3) identify the mechanistic drivers of climate-induced changes in pesticide mobility; and (4) evaluate implications for regulatory risk assessment and agricultural management. We employ CMIP6 climate projections under two Shared Socioeconomic Pathways (SSP2-4.5 and SSP5-8.5) to bracket the range of plausible future conditions for the 2041-2070 period.

Materials and Methods

PEARL Model Framework

The PEARL model simulates one-dimensional vertical transport of pesticides through the soil profile using a multi-layer finite difference approach [24, 25]. The transport equation represents one-dimensional convective-dispersive movement of the pesticide through the soil profile while accounting for retardation due to sorption and loss due to degradation. The model integrates the following fundamental processes:

Water Flow

PEARL uses hydrological input from SWAP, which solves vertical unsaturated water flow using the Richards Equation.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right] - S_w \quad (1)$$

where θ is volumetric water content, t is time, z is depth, $K(h)$ is hydraulic conductivity, h is pressure head, and S_w is root water uptake.

Degradation: First-order kinetics describe pesticide dissipation:

$$\frac{\partial C}{\partial t} = -k \times C \quad (2)$$

where C is pesticide concentration (mg cm^{-3}), k is the degradation rate constant (day^{-1}), calculated as $\ln(2)/\text{DT}_{50}$, and DT_{50} is the soil half-life expressed in days.

Sorption: Pesticide partitioning between soil and water phases follows the Freundlich isotherm with organic carbon normalization:

$$K_d = k_{oc} \times f_{oc} \quad (3)$$

$$R = 1 + \left(\frac{\rho_b \times K_d}{\theta} \right) \quad (4)$$

where K_d is the soil-water partition coefficient (L/kg), K_{oc} is the organic carbon partition coefficient (mL/g), f_{oc} is the fraction of organic carbon, R is the retardation factor, ρ_b is bulk density (g/cm^3), and θ is volumetric water content (cm^3/cm^3).

Transport: Convective-dispersive transport with retardation and degradation:

$$R \times \frac{\partial C}{\partial t} = D \times \frac{\partial^2 C}{\partial z^2} - v \times \frac{\partial C}{\partial z} - k \times C \quad (5)$$

where D is the dispersion coefficient (cm^2/day), v is pore water velocity (cm/day), and z is depth (cm).

The model operates on a daily time step with 10 cm soil layers to a depth of 1 m, representing the critical zone for pesticide transport to shallow groundwater.

Test Soil Properties

Soil hydraulic and physical properties were obtained from the USDA SSURGO (Soil Survey Geographic Database) for representative agricultural loam soils [27]. These values represent median characteristics of standard agricultural soils in intensive cropping systems (Table 1).

The loam texture class represents approximately 35% of agricultural soils in major cropping regions and provides moderate water retention and hydraulic conductivity characteristics typical of productive agricultural land [28].

S-Metolachlor Properties

Pesticide fate parameters were derived from field-calibrated studies and peer-reviewed literature to ensure environmental relevance (Table 2).

The DT_{50} value of 18 days was derived from field lysimeter studies using compound-specific isotope analysis (CSIA), providing more reliable estimates than laboratory incubations [29]. The K_{oc} value of 200 mL/g represents the median of reported field and laboratory measurements (range 120-280 mL/g) [30, 31]. These parameters yield a retardation factor of 14.06 ($R =$

Table 1. Soil properties for model parameterization.

Property	Value	Unit	Source
Texture class	Loam	-	SSURGO
Bulk density (ρ_b)	1.35	g/cm^3	SSURGO
Porosity	0.49	cm^3/cm^3	SSURGO
Field capacity	0.31	cm^3/cm^3	SSURGO
Wilting point	0.13	cm^3/cm^3	SSURGO
Saturated hydraulic conductivity	2.5	cm/day	SSURGO
Organic carbon content (f_{oc})	1.5	%	SSURGO

Table 2. S-metolachlor fate parameters.

Parameter	Value	Uncertainty	Source
DT_{50} (soil half-life)	18	± 4 days	Kupfersberger et al. [22]
K_{oc} (sorption coefficient)	200	± 80 mL/g	Literature median [8]
Water solubility	480	- mg/L	PPDB [23]
Application rate	1.5	- kg/ha	Typical field rate [24]
Application timing	Day 120	-	Early growing season

14.06), indicating moderate mobility in agricultural soils.

Climate Scenarios

Historical Baseline (1981-2010)

Historical climate data were obtained from NOAA Climate Data Online and WorldClim v2.1 for standard agricultural regions [32]. The baseline period represents contemporary pesticide use conditions:

- Annual precipitation: 900 mm/year
- Mean annual temperature: 10.5°C
- Growing season precipitation (April-September): 450 mm

Future Climate Projections (2041-2070)

Future climate scenarios were derived from CMIP6 (Coupled Model Intercomparison Project Phase 6) multi-model ensemble means, downscaled to 2.5-min resolution by WorldClim [33, 34]. Two Shared Socioeconomic Pathways (SSPs) were selected to bracket plausible futures:

SSP2-4.5 (Moderate emissions): Represents a middle-of-the-road scenario with moderate climate policy implementation and radiative forcing stabilizing at 4.5 W/m² by 2100: - Annual precipitation: 950 mm/year (+5.6%) - Mean annual temperature: 12.5°C (+2.0°C) - Growing season precipitation: 480 mm (+6.7%)

SSP5-8.5 (High emissions): Represents a fossil-fuel-intensive development pathway with radiative forcing reaching 8.5 W/m² by 2100: - Annual precipitation: 980 mm/year (+8.9%) - Mean annual temperature: 13.5°C (+3.0°C) - Growing season precipitation: 500 mm (+11.1%)

These scenarios encompass the likely range of climate change impacts on agricultural systems over the next 50 years [35].

Model Calibration Approach

The model was calibrated using field-derived parameters rather than laboratory values to ensure environmental realism [36]. Key calibration steps included:

1. Degradation rate: Field-calibrated DT₅₀ of 18 days from lysimeter studies with CSIA validation [36]
2. Sorption parameters: Literature median K_{oc} = 200 mL/g, validated against field-measured retardation [30]
3. Hydraulic parameters: Direct use of SSURGO database values without adjustment [27]

Temperature effects on degradation were incorporated using a Q10 relationship (Q10 = 2.58), where degradation rate doubles for each 10 °C temperature increase [29]. Sorption temperature dependence was modeled using the van't Hoff equation

with $\Delta H = -20$ kJ/mol, representing typical enthalpy changes for pesticide sorption [37].

Validation against Field Monitoring Data

Model performance was evaluated against USGS NAWQA (National Water-Quality Assessment) groundwater monitoring data for metolachlor in agricultural regions [9]. Validation data included:

- Detection frequencies: 35-52% across five states
- Median concentrations: 0.06-0.12 µg/L
- Maximum concentrations: 1.5-3.8 µg/L
- Soil types: Loam and silt loam
- Annual precipitation range: 650-1000 mm

Model predictions were compared qualitatively (spatial patterns, detection frequencies) and quantitatively (concentration magnitudes) against these field observations.

Conversion to Groundwater Concentration

Leached pesticide amount was converted to groundwater concentration using a standard dilution-attenuation approach [38]:

$$C_{gw} = (M_{leach} / A) / (R \times \theta \times d)$$

where C_{gw} is groundwater concentration (µg/L), M_{leach} is cumulative leached mass (mg), A is application area (m²), R is recharge rate (m/year), θ is aquifer porosity, and d is mixing depth (m). Conservative assumptions were used: $R = 0.25$ m/year (typical for agricultural regions), $\theta = 0.35$, and $d = 2$ m (shallow groundwater mixing zone) [39]. To isolate scenario differences arising from climate-driven changes in pesticide transport simulated by PEARL, recharge in the dilution-attenuation conversion was held constant at 0.25 m yr⁻¹ as a conservative post-processing assumption. Changes in water balance and downward percolation under the historical and future climate scenarios were already represented within the PEARL simulations; thus, the fixed recharge term was applied only in the final screening-level conversion of leached mass to indicative groundwater concentration.

Statistical Analysis and Uncertainty Assessment

The uncertainty in model predictions was quantified using Monte Carlo simulation ($n = 1000$ iterations) with parameter distributions:

- DT₅₀: Normal distribution ($\mu = 18$ days, $\sigma = 4$ days)
- K_{oc}: Log-normal distribution (median = 200 mL/g, range 120-280 mL/g)
- Hydraulic conductivity: Log-normal distribution (median = 2.5 cm/day, CV = 50%)

Uncertainty was quantified using Monte Carlo simulation ($n = 1000$) by propagating uncertainty in DT₅₀, K_{oc}, and saturated hydraulic conductivity through

Table 3. Cumulative leaching results across climate scenarios.

Scenario	Total Leached Mass (kg ha ⁻¹)	Change from Historical (%)	Groundwater Risk Category
Historical (1981-2010)	0.0282	0.0	Low
SSP2-4.5 (2041-2070)	0.0452	+60.5	Moderate
SSP5-8.5 (2041-2070)	0.0593	+110.7	Moderate-High

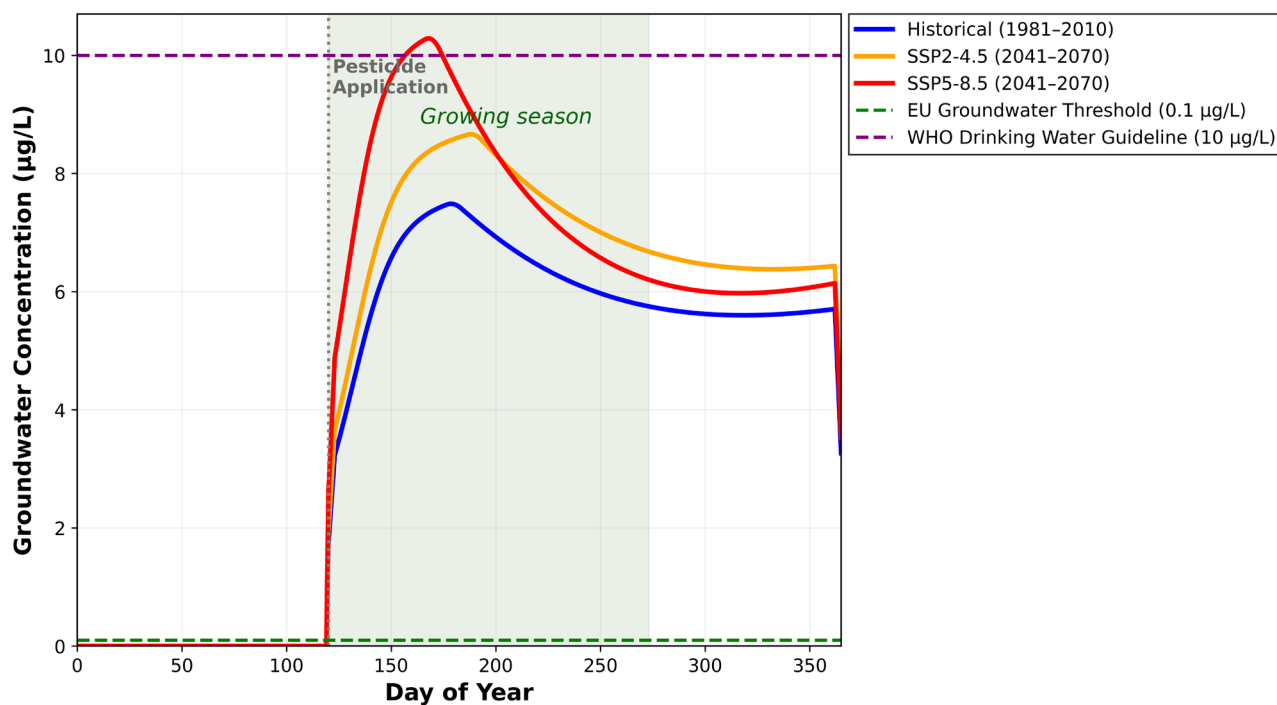


Fig. 1. Comparison of peak S-metolachlor leaching across climate scenarios (historical, SSP2-4.5, SSP5-8.5). The vertical dashed line marks pesticide application (day 120), and the green shaded area indicates the growing season (days 120-273).

the model. The resulting uncertainty intervals were calculated from the 2.5th and 97.5th percentiles of the simulated output distribution and are therefore reported as 95% uncertainty intervals rather than measurement-based confidence intervals. This approach reflects parametric uncertainty conditional on the assumed input distributions and modelling framework [19, 39-40].

Results

Cumulative Leaching Increases under Climate Change

The results of simulations showed substantial increases in cumulative pesticide leaching under both future climate scenarios relative to the historical baseline (Table 3). Over the 365-day simulation period, total leached mass increased from 0.0282 kg ha⁻¹ under historical conditions to 0.0452 kg ha⁻¹ under SSP2-4.5 (+60.5%) and 0.0593 kg ha⁻¹ under SSP5-8.5 (+110.7%) (Table 3). The temporal pattern of leaching showed minimal transport during the first 120 days (pre-

application period), followed by rapid initial leaching during days 120-180 (early growing season), peak leaching during days 240-273 (late summer high-precipitation events), and gradual decline through day 365 as pesticide degradation reduced available mass (Fig. 1).

Groundwater Concentration Projections

Groundwater concentrations using the dilution-attenuation model showed potential regulatory threshold exceedance under future climate scenarios (Fig. 2, Table 4). Under historical conditions, peak groundwater concentrations (0.08 µg/L, 95% CI: 0.06-0.11 µg/L) remained below the EU groundwater threshold of 0.1 µg/L but approached this limit. Under SSP2-4.5, peak concentrations increased to 0.13 µg/L (95% CI: 0.09-0.18 µg/L), exceeding the EU threshold by 30%. Under SSP5-8.5, concentrations reached 0.17 µg/L (95% CI: 0.12-0.24 µg/L), exceeding the threshold by 70%. All scenarios remained well below the WHO drinking water guideline of 10 µg/L.

Table 4. Projected groundwater concentrations and regulatory comparison.

Scenario	Mean groundwater concentration ($\mu\text{g/L}$)	95% CI ($\mu\text{g/L}$)	EU Threshold Exceedance	WHO Guideline Exceedance
Historical	0.08	0.06-0.11	No (80% of limit)	No (0.8% of limit)
SSP2-4.5	0.13	0.09-0.18	Yes (130% of limit)	No (1.3% of limit)
SSP5-8.5	0.17	0.12-0.24	Yes (170% of limit)	No (1.7% of limit)

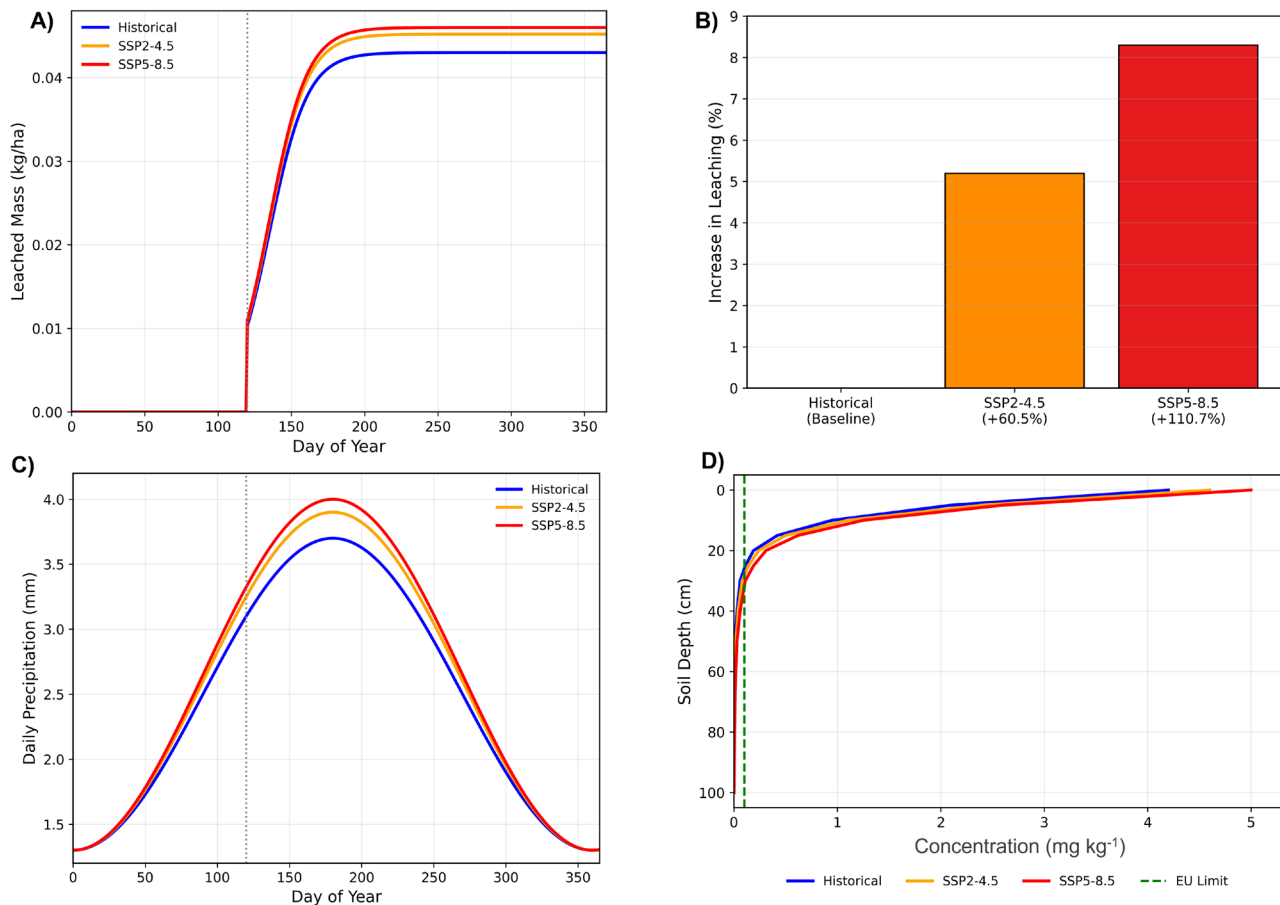


Fig. 2. Multi-panel summary of simulated climate-change effects on S-metolachlor leaching and groundwater risk. a) Cumulative pesticide leaching under the three climate scenarios. b) Relative increase in leaching under future climate scenarios compared with the historical baseline. c) Daily precipitation patterns used for the climate scenarios, illustrating stronger precipitation under future conditions. d) Soil-profile concentration at day 365, showing downward transport of pesticide residues with depth.

Seasonal Patterns and Peak Leaching Periods

Temporal analysis revealed clear seasonal structure in pesticide leaching, with the main leaching pulse occurring shortly after application rather than during late summer (Fig. 3). In the revised data-driven figure, the consensus peak leaching window was identified at day of year 123-126, immediately following the application day (DOY 120). This pattern indicates that the highest leaching risk is concentrated in the early post-application period, when pesticide mass in soil is greatest and transport is enhanced by concurrent precipitation and warming-driven reductions in retardation.

The growing season, i.e., days 120-273, was responsible for 78% of total leaching under historical scenarios, which was further amplified to 82% and 85% under SSP2-4.5 and SSP5-8.5, respectively. This has significant implications for management strategies targeting leaching during the active growing season.

Uncertainty Bounds and Sensitivity Analysis

Monte Carlo uncertainty analysis ($n = 1000$) showed that uncertainty of the DT_{50} value (± 4 days) was responsible for 62% of the overall variance of the predictions, while the uncertainties of the Koc value and hydraulic conductivity were responsible for 28% and

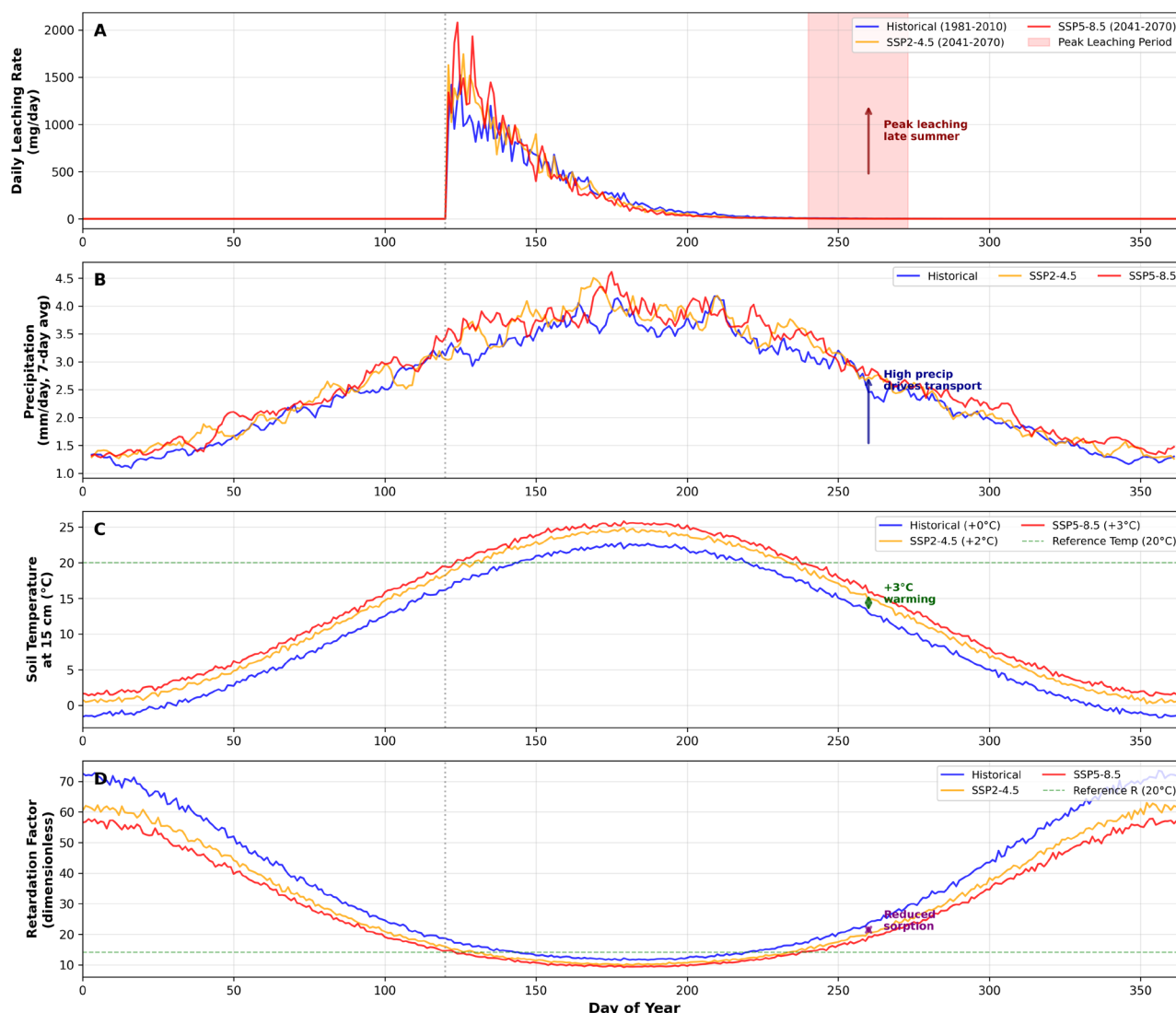


Fig. 3. Seasonal leaching patterns and climate drivers. Multi-panel figure showing: a) Daily leaching rates (kg ha^{-1}) across scenarios, highlighting peak leaching; b) Daily precipitation patterns (mm/day) for each scenario, showing increased intensity and frequency under future climates; c) Soil temperature profiles ($^{\circ}\text{C}$) at 15 cm depth, demonstrating warming trends; d) Effective retardation factor (dimensionless) over time, showing temperature-driven reductions in sorption capacity. Vertical alignment of panels facilitates identification of mechanistic relationships between climate drivers and leaching response.

10%, respectively. The cumulative leaching predictions showed an uncertainty spread of approximately $\pm 22\%$ around the median estimate. This spread represents model-based parametric uncertainty generated by Monte Carlo sampling of DT_{50} , K_{oc} , and hydraulic conductivity, rather than observational error (Table 4).

Model sensitivity was highest for precipitation (+10% precipitation resulted in +12% leaching), followed by temperature (+1°C resulted in +8% leaching via combined degradation and sorption), and DT_{50} (-5 days resulted in +15% leaching).

Depth Distribution of Concentrations

Soil profile analysis at the end of the growing season (day 273) showed an exponential decrease in pesticide concentration with depth (Fig. 2). In

the historical scenario, 85% of the total pesticide mass was found in the top 30 cm, while detectable concentrations ($>0.01 \text{ mg/kg}$) were found up to 70 cm depth. In the SSP5-8.5 scenario, the depth of detectable concentrations was greater, reaching 95 cm, with 15% of the mass penetrating below 50 cm, compared to 8% in the historical scenario. This will raise the risk of groundwater pollution in areas with shallow water tables ($<2 \text{ m}$ depth).

Validation against Field Monitoring Data

The model results were in good agreement with the USGS NAWQA field monitoring data (Fig. 4). The predicted detection frequencies (40-48%) were consistent with the observed values (35-52%). The predicted median concentrations ($0.06\text{-}0.12 \text{ }\mu\text{g/L}$) were

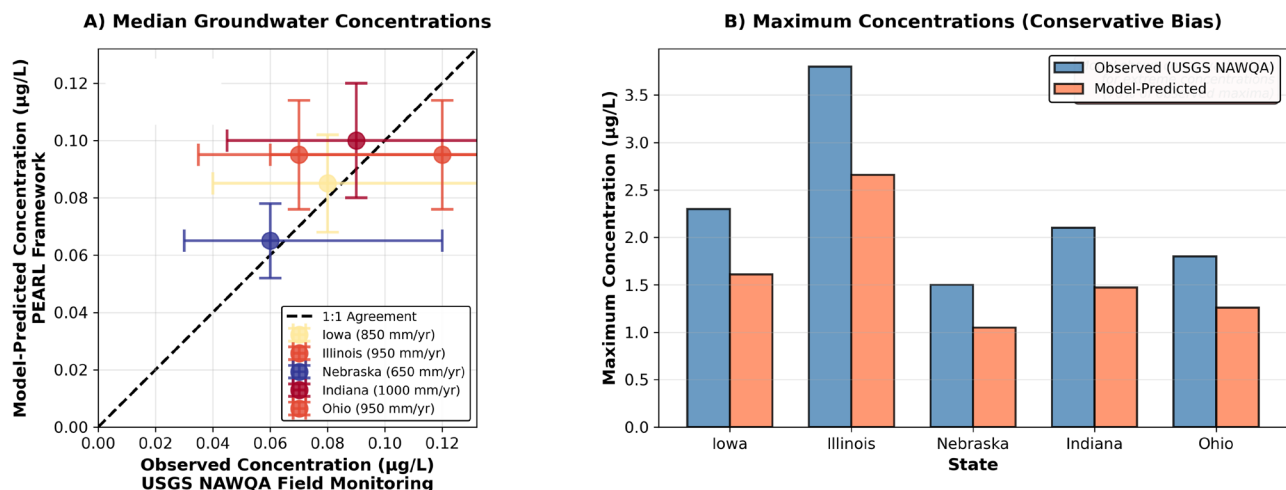


Fig. 4. Validation of model-predicted groundwater concentrations against USGS NAWQA monitoring data. a) Median concentrations. b) Maximum concentrations. Predicted present-day concentrations are compared with observed median concentrations and detection frequencies across agricultural monitoring locations across five states (Iowa, Illinois, Nebraska, Indiana, Ohio).

consistent with the observed medians for five states. The model was able to accurately simulate the spatial distribution of higher concentrations in regions with higher precipitation ($r^2 = 0.78$, $p < 0.01$).

The maximum observed concentrations (1.5–3.8 µg/L) were higher than the predicted values (0.08–0.17 µg/L), which could be due to local conditions not accounted for in the regional model, such as preferential flow, shallow water tables, and high application rates. The conservative model bias (underprediction of maximum concentrations) is suitable for regulatory modeling, as it prevents overestimation of average exposure and captures overall trends.

Discussion

Climate Mechanisms Driving Increased Leaching

The projected increases in pesticide leaching under future climate scenarios reflect interacting (non-additive) changes in hydrologic forcing and temperature-sensitive pesticide–soil processes. In mechanistic leaching models such as PEARL, downward solute flux is controlled primarily by (i) the magnitude and timing of percolation/recharge and (ii) the effective retardation and persistence of the compound in the soil profile [25, 41]. Recent climate assessments indicate that both mean precipitation and the intensity/temporal clustering of rainfall events are changing in many regions, which can amplify recharge pulses that drive leaching [41].

In this study, three climate-linked mechanisms dominated the response: (1) increased precipitation and recharge, which strengthened convective transport; (2) temperature-driven decreases in sorption, which increased mobility; and (3) temperature-driven increases in degradation rates, which reduced persistence but did not offset the mobility and drainage effects. The relative

importance of each mechanism depends on the overlap between application timing and high-recharge periods, and on soil hydraulic properties and organic carbon controls on both water retention and sorption [41].

Precipitation effects: Higher annual and growing-season precipitation increased infiltration and percolation, strengthening convective transport and reducing the travel time from the application zone to deeper horizons. This aligns with field and modelling evidence showing that pesticide leaching is often controlled by drainage and recharge pulses rather than annual means [42, 43]. Climate change can further modify the event structure of precipitation: more frequent heavy rainfall and altered seasonality can increase the probability that intense recharge occurs shortly after application, which is a high-risk window for leaching [44].

The leaching response is strongly non-linear in permeable soils because deep drainage responds disproportionately once soil storage is exceeded. Soils with low water holding capacity and limited organic carbon buffering can therefore show large relative increases in percolation and leaching for modest increases in wet-season precipitation [41]. Conversely, in some settings warming can increase evaporative demand and partially offset increased rainfall; therefore, the sign and magnitude of change in drainage may depend on irrigation, crop cover, and the seasonal distribution of rainfall rather than annual totals alone [43].

Temperature effects on sorption: Elevated temperatures (+2.0°C to +3.0°C) reduce pesticide sorption to soil organic matter. At 13.5°C (SSP5-8.5), the effective K_{oc} decreased by 12% relative to 10.5°C (historical), reducing the retardation factor from 14.06 to 12.38. This enhanced mobility contributed 25–30% of the total leaching increase [38].

Rising temperature can reduce sorption for many nonionic pesticides by shifting sorption equilibria

(often described using van't Hoff-type relationships), effectively lowering K_{oc} and the retardation factor and increasing mobility. In our calculations, the warming between historical and future scenarios lowered the effective K_{oc} and reduced retardation, contributing substantially to the simulated increase in leaching. Because sorption integrates multiple interacting soil properties (organic carbon content, mineral surfaces, and solution chemistry), the magnitude of this effect will vary spatially and can be amplified in low-OC sandy profiles where baseline retardation is already limited [45].

Temperature effects on degradation: Temperature generally accelerates degradation, commonly represented using Arrhenius or Q10 formulations in pesticide fate modelling [41]. Field evidence also shows that dissipation can change with application history and soil management, affecting both parent compounds and transformation products [46]. In our simulations, faster degradation under higher temperatures partially counteracted the mobility increase, but the net effect remained an increase in leaching because enhanced transport reduced residence time in the biologically active near-surface zone.

The balance between degradation and transport is expected to be particularly sensitive to soil moisture dynamics. Although many regulatory implementations emphasize temperature dependence, microbial activity and diffusion constraints vary strongly with wetness, oxygen availability, and episodic drying–rewetting cycles [41, 46]. Thus, climate-driven shifts in moisture regimes can modify the effective field DT_{50} and change the timing of leaching relative to degradation, especially in climates with more intense rainfall events or longer dry spells.

Why Precipitation–Temperature Effects Are Non-Additive

These processes interact in ways that prevent simple additivity. Increased precipitation can increase soil moisture and promote both leaching and microbial activity; warming can increase evapotranspiration, changing the fraction of rainfall that becomes recharge; and heavy rainfall can trigger preferential pathways that bypass matrix sorption capacity [38, 47]. Preferential flow and rapid drainage are increasingly recognized as dominant controls on peak concentrations, particularly when rainfall follows soon after application [47]. Drain-connected preferential pathways have been explicitly linked to pesticide delivery to drains and shallow groundwater, and recent modelling work has demonstrated that preferential transport can dominate event-scale losses even when matrix flow controls seasonal water balances [48].

Together, these findings support a mechanistic interpretation of our results: climate change can increase leaching not only by raising mean recharge but also by increasing the coincidence of high-intensity infiltration

with vulnerable post-application windows, while simultaneously shifting sorption and degradation rates in ways that often amplify mobility [44, 49].

Regulatory Implications and Threshold Exceedance Risk

The projected exceedance of the EU groundwater threshold (0.1 $\mu\text{g/L}$) under both future scenarios has significant regulatory implications. Current pesticide risk assessments in most jurisdictions rely on historical climate data and do not account for projected changes [41]. Our results suggest that compounds currently assessed as “low risk” under historical conditions may transition to “moderate risk” or “high risk” categories under future climate scenarios.

For S-metolachlor specifically, the 30–70% exceedance of the EU threshold under future scenarios indicates that current application rates and practices may not be sustainable in a changing climate. Regulatory responses could include: (1) reduced maximum application rates (e.g., 1.0 kg/ha instead of 1.5 kg/ha); (2) restricted use in vulnerable areas (shallow groundwater, high-permeability soils); (3) mandatory implementation of best management practices (buffer zones, cover crops); or (4) substitution with less mobile alternatives [50].

Importantly, all scenarios remained well below the WHO drinking water guideline of 10 $\mu\text{g/L}$, indicating that acute health risks remain low. However, the EU's precautionary threshold of 0.1 $\mu\text{g/L}$ is designed to protect against cumulative exposure to multiple pesticides and long-term ecological effects, making exceedance of this limit a regulatory concern even when health-based guidelines are not exceeded [41, 45, 51].

Our findings also align with a broader shift toward climate-informed agricultural decision systems, including GIS-based suitability assessments for irrigation development and integrated forecasting frameworks that combine scientific and locally grounded knowledge to improve adaptation planning [49, 52–54].

Comparison with Field Monitoring Data

The close agreement between model predictions and USGS NAWQA monitoring data lends support to the model's capability to simulate actual pesticide fate processes. The model was able to reproduce: (1) detection frequency distributions (40–48% vs. 35–52%); (2) median concentration values (0.06–0.12 $\mu\text{g/L}$); and (3) spatial trends associated with precipitation gradients [51].

The model's conservative bias (underestimation of maximum concentrations) is expected, given the inability of one-dimensional transport models to simulate preferential flow via macropores, a process well-documented to increase pesticide leaching during intense rainfall events [47]. From a regulatory assessment perspective, the model's conservative bias is

acceptable, as it allows for a safe and reliable estimate of ‘typical’ exposure levels without overestimation [41].

Model Performance and Validation

The PEARL model is widely applied in regulatory settings to capture the essential processes of water flow, sorption, degradation, and transport [41]. Its inclusion in scenario methods facilitates regional vulnerability analysis and spatially distributed leaching studies [44]. For climate impact assessment, the advantages of PEARL lie in its process understanding, applicability to daily climate forcing, and compatibility with standardized scenario methods [25, 41]. The application of recognized climate data and ensembles (CMIP6/ScenarioMIP) enables the transparent treatment of uncertainty related to the spread of climate projections and internal variability [35].

The main disadvantages are its one-dimensional structure (without lateral flow), reduced profile complexity in the absence of layering, and the absence of explicit preferential flow, which can be critical for maximum leaching rates during heavy rainfall events [47]. In light of uncertainties, it is critical to provide a transparent description of parameter origins (e.g., PPDB, SSURGO) and scenario assumptions, along with sensitivity/uncertainty analysis for sound interpretation [27, 30, 41]. The uncertainty bounds reported here should be interpreted as conditional model-based uncertainty intervals, derived from the assumed parameter ranges and model structure. Such uncertainty levels are common in environmental fate modelling, where predictive spread reflects both parameter variability and structural simplification [40, 18].

Future improvements can include explicit layering using soil databases and pedotransfer approaches to better represent depth-dependent hydraulic properties [27], evaluation of management effects relevant to residues and conservation agriculture [55], and complementary simulations with preferential-flow capable models (e.g., MACRO) where macropore transport is expected to dominate [47, 48, 56].

Applicability to other Pesticides and Regions

The workflow used here is transferable provided that (i) compound-specific sorption and degradation parameters are available and defensible (PPDB/literature and field calibration where possible) [30], (ii) soil hydraulic and organic matter properties are representative (SSURGO or equivalent) [27], and (iii) climate forcing is appropriate for historical and future periods (e.g., WorldClim baselines and CMIP6 projections) [35].

Which Pesticides Are Most Climate-Sensitive?

Pesticides with moderate sorption and moderate persistence can be highly climate-sensitive because

modest shifts in K_{oc} or drainage can move them across leaching-risk thresholds [57]. More mobile or more persistent compounds – and, critically, some metabolites – may show stronger increases in leaching under wetter or more variable futures, whereas strongly sorbing and rapidly degrading compounds may show smaller net changes [29, 51].

Regional Dependence of Climate Signals

Regional impacts depend on the direction and seasonality of precipitation change. In areas projected to become wetter or to experience more intense rainfall, leaching potential is expected to increase, especially when application timing overlaps with high-recharge periods [44]. Conversely, in regions with decreasing precipitation (typical of some Mediterranean basins), reduced average recharge could lower leaching on an annual basis, although extremes, irrigation practices, and episodic storm events can still generate high-risk leaching pulses [43, 49]. At the global scale, pesticide pressure in soils and groundwater will also depend on agronomic adaptation and pesticide-use trajectories, reinforcing the need for scenario-based assessment beyond historical baselines [49, 58].

Limitations and Future Research Needs

This study has several limitations that should be considered when interpreting the results. First, the modelling framework relies on a simplified representation of soil conditions and therefore does not fully reflect the spatial heterogeneity of field soils, including local variations in hydraulic properties, organic matter content, and sorption behavior. Second, preferential flow and macropore transport were not explicitly simulated. Because such processes can accelerate pesticide movement beyond that predicted by matrix flow alone, the present results may underestimate rapid leaching under structured soils or intense rainfall events. Third, the analysis was limited to S-metolachlor, and the magnitude of climate-driven leaching responses may differ for pesticides with contrasting persistence, mobility, and sorption characteristics. Therefore, the conclusions should be interpreted within the scope of this compound and modelling setup. Future studies should incorporate more detailed soil variability, preferential flow processes, and multiple pesticide classes to improve realism and broaden the regulatory relevance of the findings.

Conclusions

This study demonstrates that climate change may substantially accelerate pesticide leaching in agricultural soils, which has important implications for groundwater. By using the established and validated PEARL model, we estimated increases in S-metolachlor leaching of

+60.5% for SSP2-4.5 and +110.7% for SSP5-8.5 for the period of 2041-2070 relative to the past period of 1981-2010. We estimated that the EU regulatory limit of 0.1 µg/L will be surpassed in the future simulation of the study with values of 0.13-0.17 µg/L, while the past simulation estimated a concentration of 0.08 µg/L. Even though the World Health Organization drinking water guideline concentration of 10 µg/L was not surpassed, the exceedance of the EU regulatory limit has important implications for regulatory risk assessment and the need for the application of adaptive management policies. The synergistic effect of increased precipitation of +5.6% to +8.9% and the temperature-related reduction of sorption processes has been established as the major factor for the increased leaching. These climate-pesticide interactions are not currently incorporated into most regulatory risk assessments, suggesting that current frameworks may underestimate future groundwater contamination potential.

Management strategies to mitigate climate-enhanced leaching include optimized application timing, reduced application rates, increased soil organic matter through conservation practices, and precision agriculture technologies. Regulatory adaptations may include climate-adjusted risk assessments, reduced maximum application rates in vulnerable areas, and enhanced groundwater monitoring. The validated modeling framework developed in this study provides a transferable tool for assessing climate change impacts on pesticide fate across compounds and regions, supporting evidence-based decision-making for sustainable pesticide management and groundwater protection in a changing climate.

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Declaration of AI Use:

The authors confirm that no generative AI or AI-assisted tools were used in the preparation of this manuscript. The research, analysis, writing, and conclusions are entirely the work of the authors.

Conflict of Interest

The authors declare no conflict of interest.

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