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Simulation and Prediction of PCBs in Seven Regions Using BETR-GLOBAL and Random Forest

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Abstract

An integrated model approaching to combining the BETR-GLOBAL model with a Random Forest method was developed in this research. Firstly, the BETR-GLOBAL model was employed to simulate the spatial and temporal distribution of PCBs concentrations in seven representative regions from 2001 to 2010. These simulation results were used to train a Random Forest regression model to predict the trend of PCBs concentrations from 2031 to 2040. In addition, Spearman's rank correlation coefficient was applied to evaluate the relationships between PCBs pollution levels across different regions. The results show that the future trends in PCBs concentrations could effectively predicted from this method and correlations between regional pollution levels were revealed. Moreover, that PCBs are likely to persist and accumulate in the environment throughout 2031-2040 was found in the research, reflecting a spatiotemporal lag in their declines. A scientific reference may be served from the findings of this research and data supporting the control of PCBs pollution and the formulation of regional environmental policies were provided in this article.

Keywords

PCBs, Random Forest, BETR-GLOBAL

1. Introduction

Polychlorinated Biphenyls (PCBs), a typical class of Persistent Organic Pollutants (POPs), have been characterized by their chemical stability, electrical insulating properties, and thermal resistance (Akhtar et al., 2021). Since the 1930s, the PCBs have been widely used in the various fields of industry, including transformer oils, capacitors, and plastic additives (Albraihi et al., 2023). Due to their persistence and volatility, the PCBs have been recognized as environmentally hazardous substances (Wu et al., 2022). As a result of their persistence and volatility, the PCBs have been identified as hazardous pollutants (Zhu et al., 2022; Othman et al., 2022; Ravanipour et al., 2022), and the PCBs were also designated as one of the first priority-controlled persistent organic pollutants (POPs) under the Stockholm Convention (Akinrinade et al., 2024). In recent years, much research on the PCBs pollutions has been increasingly advanced on a global scale, particularly in source apportionment, environmental trends, and risk assessment. the major sources of PCBs, such as industrial emissions, have been effectively identified through the application of multivariate statistical methods in terms of source apportionment, including Positive Matrix Factorization (PMF) (Han et al., 2023), heavy metals (Feng et al., 2023), coal and wood burning (Srivastava et al., 2021). For example, in the Beiluo River Basin of Shanxi Province, China, the main sources of PCBs were identified as industrial emissions, technical mixtures, and coal and wood combustion (Wang et al., 2023). In addition, more research, in Guiyu Town of Guangdong Province, indicated that both traditional and emerging electronic waste recycling activities have significantly influenced the distribution of PCBs in local soils and water bodies (Liu et al., 2022). In terms of environmental trends, the results of research have shown that although the production of PCBs has been banned in most countries, their stability and persistence in the environment have led to continued release from old equipment and waste materials (Fazari et al., 2024). Moreover, the PCBs could be transmitted long distances through the atmosphere, leading to their detection even in regions far from the emission sources. For example, the significant temporal and spatial changes in PCBs concentrations were found from the results of research in Chinese mainland during 1960-2019 (Li et al., 2023b). In terms of risk assessment, the potential risks of the PCBs to ecosystems and human health have been further evaluated. For instance, the PCBs concentrations detected in soils near an industrial park in Northwest China have been indicated as a potential carcinogenic risk (Li et al., 2023a). Additionally, the PCBs levels in the breast milk of primiparous women living near incinerators were investigated in a study in the UK (Parsons et al., 2025). Although preliminary results did not show a direct correlation with proximity to incinerators, further analysis revealed that an association between the distribution of environmental particulates and pollutant levels was found. Multiple field observations and simulation studies have shown that a strong long-range atmospheric transport (LRAT) capability of PCBs exists, allowing them to spread onto remote regions such as the Arctic and marine ecosystems, causing global ecological pollution (Hung et al., 2022). However, gaps remain in the understanding of global-scale migration pathways and spatiotemporal evolution characteristics of the PCBs concentrations (Pan et al., 2025; Zhang et al., 2024; Savage et al., 2024), particularly in the simulation and prediction of future concentration trends. Current research has been mostly focused on regional or national scales, and systematic simulations of the spatiotemporal dynamics of PCBs in global multimedia systems are lacking. Moreover, traditional models, such as regional *multi*-compartment models, often rely on static input parameters and struggle to fully capture the nonlinear relationships and complex interactions involved in pollutant migration processes (Meierdierks et al., 2022). In addition, there is a lack of data-driven methods with predictive capabilities to support projections of the PCBs pollution trends beyond 2030, particularly in the diffusion pathways of rapidly industrializing countries (Eze et al., 2024; Yu et al., 2024). These research gaps are gradually being filled in the context of increasing global environmental governance pressures. The conventional BETR model is known to have limitations, such as a traditional model structure, strong fixed parameters, and difficulty in integrating with machine learning methods like random forests and neural networks (MacLeod et al., 2011). To address these limitations, a global simulation model based on multimedia pollutant migration—BETR-GLOBAL (Berkeley-Trent Global Contaminant Fate Model) (Chen et al., 2024; Meena & Qureshi, 2025; Luo et al., 2024; Vudamala et al., 2024)—has been introduced in this research. The globe is divided into 288 *multi*-media regions, covering major environmental media, including air, water, soil, and sediments, and the cross-region migration, transformation, and accumulation processes of pollutants could be simulated. To address the issue of pollution trend prediction, the Random Forest (RF) machine learning method (He et al., 2022; Wang et al., 2021), has been incorporated into this research, leveraging its strengths in variable selection and prediction to develop a forecasting framework. Specifically, the current research targets seven representative global regions, where the spatiotemporal distribution of PCBs concentrations from 2001 to 2010 is initially simulated using BETR-GLOBAL. Subsequently, the RF method, along with meteorological factors, was applied to forecast the evolution of PCBs concentrations from 2031 to 2040. Moreover, the pollutions between regions, revealing the structural and evolutionary patterns of global pollution diffusion pathways, were investigated in the research.

This research aims to achieve the following two objectives: (1) to simulate PCBs concentrations from 2001 to 2010 using the BETR-GLOBAL model and to predict PCBs concentrations for 2031 to 2040 using the Random Forest method; (2) to analyze the correlation of PCBs pollution levels across different regions, thereby providing data support and theoretical reference for global PCBs management and regional environmental policy development.

2. Methods

2.1. Model

The BETR-GLOBAL model was used to simulate the global transmission of PCBs in 288 multimedia regions (**Figure 1**). The seven representative regions (regions 37, 57, 60, 63, 86, 94 and 133) selected in this study are mainly based on the following points: they cover different geographical regions around the world and are spatially representative; the pollution concentration levels vary greatly, covering high, medium and low pollution areas; the intensity of human activities in the region is different, which is conducive to analyzing the relationship between pollution and human activities.

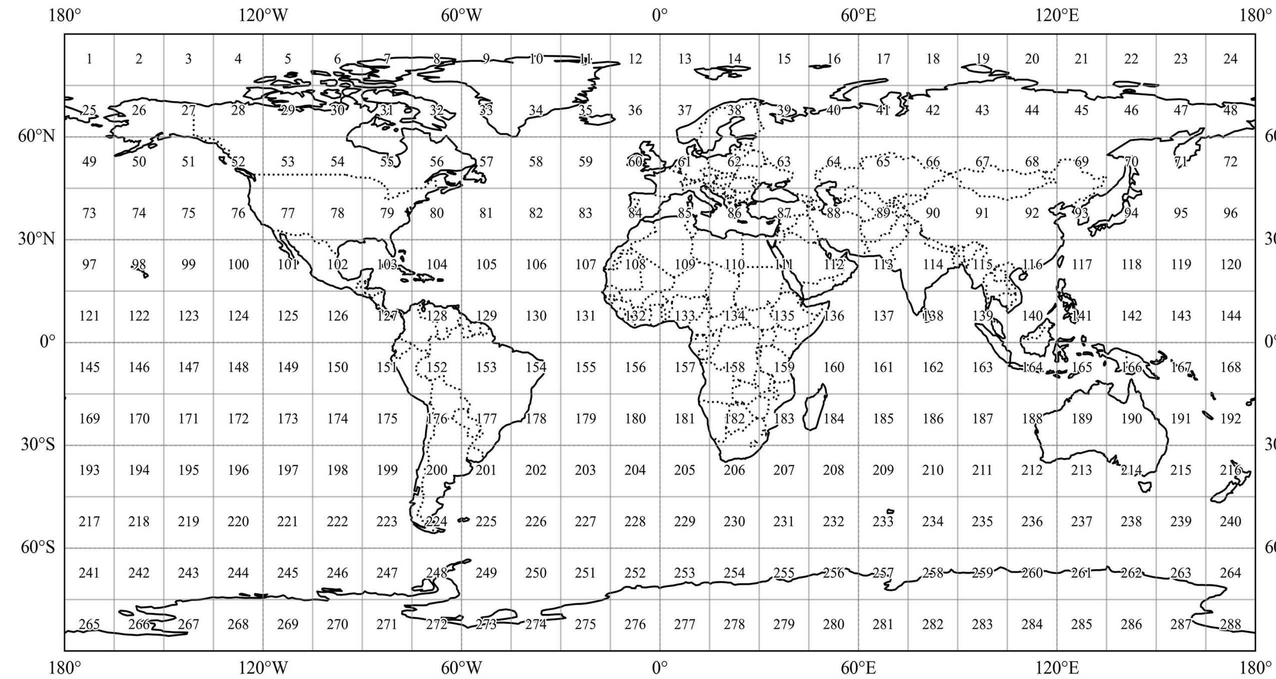

Figure 1. Global distribution map of 288 regions in the BETR model.

2.2. Methodology

In this research, the BETR-GLOBAL model was used to simulate the distribution of PCBs concentrations. The model divides the global environment into 288 regions. Simulations were conducted for seven representative regions worldwide during the period from 2001 to 2010, and the spatiotemporal evolution of PCBs concentrations in these regions was obtained. The random forest training meteorological function is used to predict the seven representative regions of the world from 2031 to 2040.

Specifically, the PCBs concentration data from 2001 to 2010, simulated by the BETR-GLOBAL model, were used as training samples. For the period of 2031-2040, meteorological functions were artificially defined, as shown in Equations (1)-(6), assuming that temperature (T), humidity (H), wind speed (W), and solar radiation (S) influence PCBs concentrations. The variation functions T(t), H(t), W(t), and S(t) were used to modify future meteorological scenarios according to Equations (1)-(4). In Equation (5), k_1, k_2, k_3 and k_4 represent the influence coefficients of temperature, humidity, wind speed, and solar radiation, respectively. $F(t)$ denotes the combined influence factor. The predicted PCBs concentration D(t) is assumed to be linearly related to F(t), as expressed in Equation (6), where a and b are coefficients representing the sensitivity of PCBs concentration to the combined factor and the baseline concentration. A Random Forest regression model was trained using the adjusted meteorological functions, and the future trend of PCBs concentrations was predicted accordingly. Since the meteorological conditions for 2031-2040 were artificially defined, the predicted concentrations reflect possible trends under specific scenarios.

To explore the correlation of PCBs pollution between different regions, Spearman's rank correlation coefficient was used, as shown in Equation (7). In this equation, d_i is the rank difference of the i^{th} regional variable, and n is the number of data points. The correlation coefficient ranges from −1 to 1, with values near 1 indicating a strong positive correlation, values near −1 indicating a strong negative correlation, and values near 0 indicating little or no correlation.

$$\mathrm{T}(t) = 20 + 10\sin\left(\frac{2\pi t}{365}\right) \tag{1}$$

$$H(t) = 50 + 20\cos\left(\frac{2\pi t}{365}\right) \tag{2}$$

$$W(t) = 2 + \sin\left(\frac{2\pi t}{365}\right) \tag{3}$$

$$S(t) = 8 + 2\cos\left(\frac{2\pi t}{365}\right) \tag{4}$$

$$F(t) = k_1 \cdot T(t) + k_2 \cdot H(t) + k_3 \cdot W(t) + k_4 \cdot S(t) \tag{5}$$

$$D(t) = a \cdot F(t) + b \tag{6}$$

$$\rho = 1 - \frac{6\sum_{i=1}^{n} \mathrm{d}_i^2}{n(n^2 - 1)} \tag{7}$$

3. Results

3.1. Modeling the Distribution Trends of PCBs Concentrations from 2001 to 2010

The data were further processed to map the spatial distribution of PCBs through BETR-GLOBAL (see Figure 2), which shows the distribution of PCBs concentration in each region over time from 2001 to 2010. It could be seen from Figure 2 that PCBs concentrations in 2006 and 2007 were relatively high. In 2006, the PCBs concentration reached 0.01 ng/m^3 in several regions, which may be attributed to large-scale industrial production and the absence of emission limits during those periods.

3.2. Prediction of PCBs Concentrations Distribution Trends from 2031 to 2040

The pollutant concentration data predicted for 2031-2040 using the Random Forest model are presented in Table 1, and the predicted concentration distribution is shown in Figure 3. It could be observed that the PCBs concentration ranges in Regions 37 and 57 exhibit relatively smooth changes, while Regions 94 and 133 show a sharp increase in PCBs concentrations in 2035 and 2036, followed by a decline beginning in 2037 and reaching a lower level by 2040.

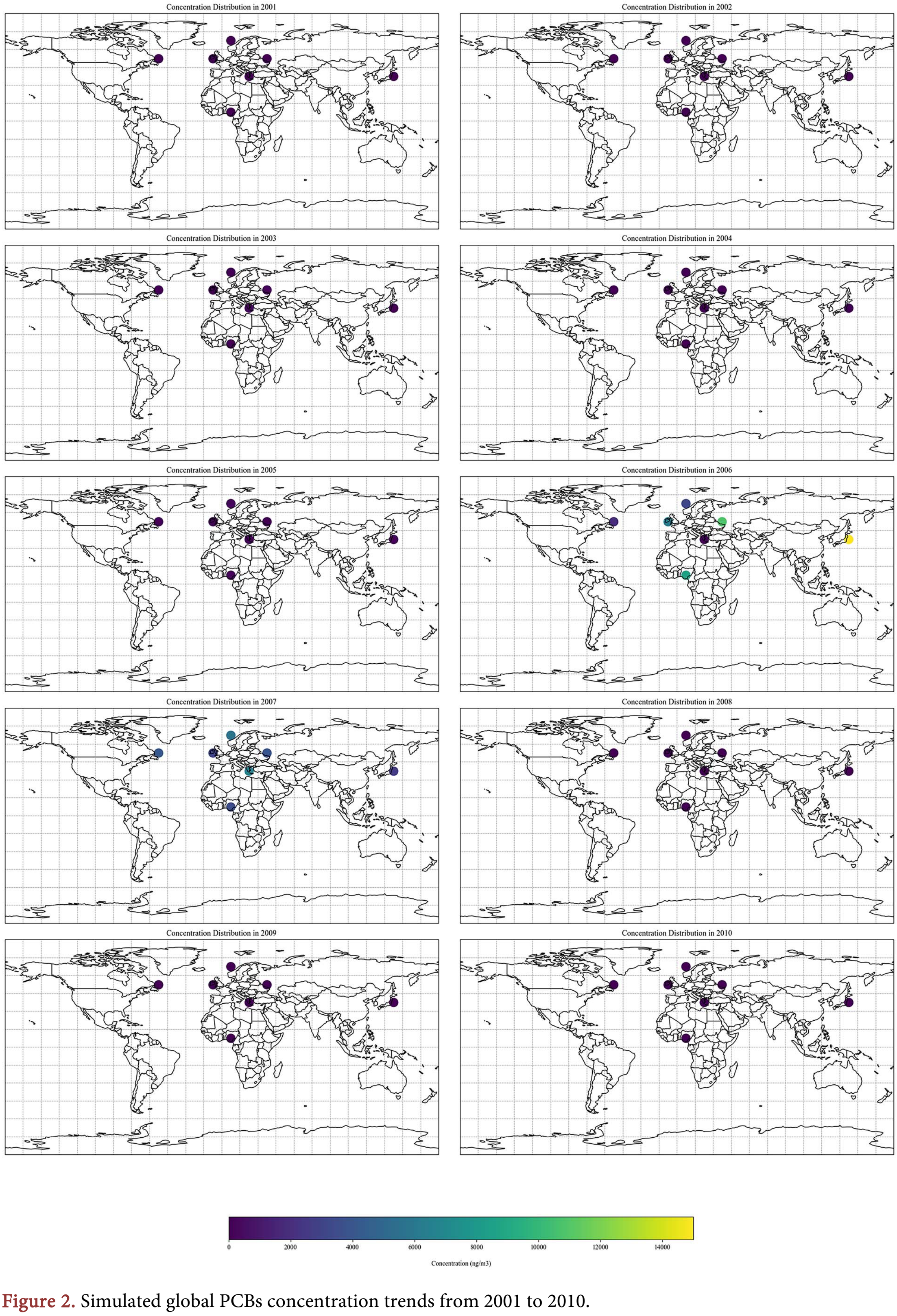

Figure 2. Simulated global PCBs concentration trends from 2001 to 2010.

Table 1. Prediction of pollutant concentration in different regions by Random Forest model with climate factors added from 2031 to 2040.

Year	Region37 (ng/m^3)	Region57 (ng/m^3)	Region60 (ng/m^3)	Region63 (ng/m^3)	Region86 (ng/m^3)	Region94 (ng/m^3)	Region133 (ng/m^3)
2031	1.86E+00	3.30E+00	1.57E+02	7.58E+01	2.18E+02	4.30E+00	5.78E+00
2032	2.06E+00	2.36E+00	1.33E+02	8.15E+01	2.18E+02	5.93E+00	8.07E+00
2033	1.88E+00	2.38E+00	1.69E+02	6.28E+01	2.47E+02	2.80E+01	5.48E+01
2034	2.05E+00	1.91E+00	8.48E+01	7.39E+01	3.34E+02	6.42E+02	4.52E+02
2035	2.08E+00	3.20E+00	7.90E+01	8.55E+01	3.81E+02	7.49E+03	3.79E+03
2036	2.16E+00	1.82E+00	2.45E+02	7.56E+01	2.17E+02	1.72E+04	1.06E+04
2037	1.97E+00	1.73E+00	3.40E+02	4.62E+01	3.02E+02	8.13E+03	6.69E+03
2038	1.86E+00	3.13E+00	8.78E+01	6.64E+01	1.18E+02	5.17E+02	9.26E+02
2039	1.88E+00	1.78E+00	1.28E+02	9.84E+01	2.85E+02	1.40E+01	1.31E+01
2040	1.71E+00	2.15E+00	1.13E+02	5.74E+01	1.58E+02	6.16E+00	5.99E+00

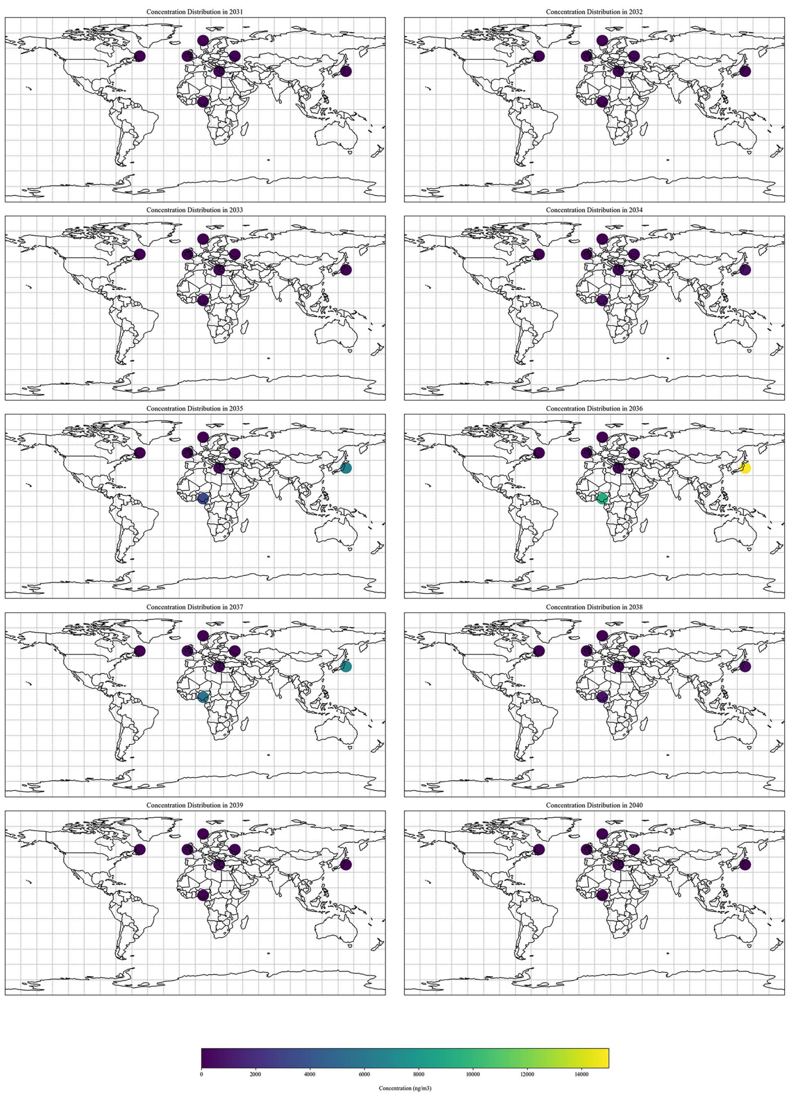

Figure 3. Forecast PCBs concentration distribution during 2031-2040.

3.3. Correlation Analysis

The Spearman rank correlation coefficient matrix of the above 7 regions predicted by the BETR-GLOBAL model is shown in Table 2. Correlation information of PCBs concentrations among the regions was provided the correlation coefficient matrix.

Table 2. Correlation coefficient matrix of different regions.

Year	Region37	Region57	Region60	Region63	Region86	Region94	Region133
Region37	1.00	−0.23	0.07	0.38	0.47	0.60	0.63
Region57	−0.23	1.00	−0.39	0.22	−0.16	−0.43	−0.37
Region60	0.07	−0.39	1.00	−0.35	−0.18	0.10	0.14
Region63	0.38	0.22	−0.35	1.00	0.27	−0.22	−0.16
Region86	0.47	−0.16	−0.18	0.27	1.00	0.32	0.25
Region94	0.60	−0.43	0.10	−0.22	0.32	1.00	0.98
Region133	0.63	−0.37	0.14	−0.16	0.25	0.98	1.00

As could be viewed from Figure 4 and be analyzed from Table 2, and the correlation coefficient between District 94 and 133 reaches 0.98, indicating a strong positive correlation exists between them; the correlation coefficient between district 37 and 133 is 0.63; the correlation coefficient between district 37 and 94 is 0.60, indicating a strong positive correlation exists between them.

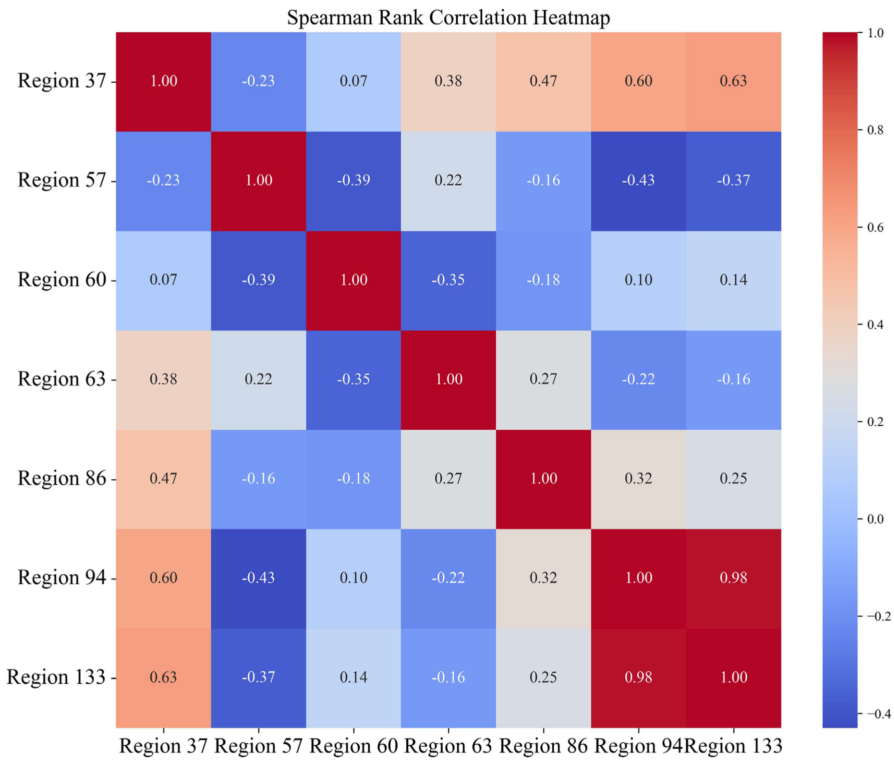

Figure 4. Seven regional heat maps.

4. Discussion

In this study, there is still a certain degree of uncertainty in the process of simulating and predicting PCBs concentrations using the BETR-GLOBAL model and the random forest (RF) method. On the one hand, the BETR-GLOBAL model simplifies some environmental media processes; on the other hand, the RF model is more sensitive to input variables, and the assumptions about future meteorological factors may also introduce errors, thus affecting the reliability of the prediction results. In addition, the meteorological function currently used can only roughly reflect the trend of climate change. Future research can introduce more sophisticated and realistic meteorological data to improve the accuracy of concentration trend simulation. Spatial analysis shows that the concentrations in areas 37 and 57 are relatively stable, which may be due to consistent environmental inputs; while areas 94 and 133 fluctuate significantly, which may be affected by local emission events, reflecting the differences in the migration paths and meteorological driving mechanisms of pollutants in different regions (Bai et al., 2022). The results of the study revealed significant spatiotemporal variability between regions (Zhang et al., 2025), which not only provides a basis for regional differentiation of pollutant control strategies, but also provides inspiration for the global management of persistent organic pollutants: in the future, cross-regional pollution control coordination should be strengthened, and multi-source observations and modeling methods should be further combined to improve the robustness of simulations and policy support.

5. Conclusion

The BETR-GLOBAL multimedia environmental model with the Random Forest machine learning approach to investigate the spatiotemporal dynamics of polychlorinated biphenyls (PCBs) across seven representative global regions was integrated in this research. The simulation results from 2001 to 2010 and the predictions for 2031 to 2040 highlighted regional differences in PCBs concentration patterns, influenced by environmental conditions and pollutant transport processes. Strong inter-regional correlations were identified, suggesting the existence of shared pollution drivers and atmospheric linkages. The combination of process-based modeling and data-driven prediction provides a robust framework for understanding and forecasting persistent organic pollutant behavior.

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Conflicts of Interest

The authors declare no conflict of interest.

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