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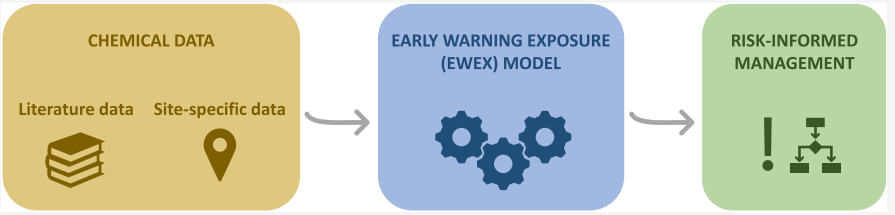
An Early Warning Exposure Assessment Framework (EWEX) for Health and Environmental Risk Evaluation Using PFAS in Indirect Potable Water Reuse Systems

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ABSTRACT: Per- and polyfluoroalkyl substances (PFAS) and industrial persistent, mobile, and toxic (iPMT) compounds pose growing risks to water quality. However, quantitative tools to prioritize compounds for remediation and evaluate exposure under varying environmental scenarios remain limited. This paper presents the first application of a Bayesian probabilistic early warning exposure assessment (EWEX) model to evaluate PFAS and iPMTs in indirect potable water reuse (IPR) systems. By integrating literature-derived and site-specific data, the model explicitly accounts for uncertainty and provides a flexible framework for scenario analysis. The model's performance was demonstrated for PFOS, trifluoromethanesulfonic acid (TFMSA), and carbamazepine (CBZ), revealing sensitivity to data quality and emphasizing the importance of robust monitoring and transferable data sets. In addition to removal via treatment processes, dilution in the environment substantially reduces contaminant concentrations, highlighting the influence of the hydrological setting and the associated climate-related environmental factors on exposure outcomes. The EWEX framework serves as a decision-support tool for utilities and regulators, facilitating risk-informed management of emerging contaminants in water reuse systems. Future work should expand the data set for poorly studied compounds, refine treatment process representations, especially for short-chain PFAS, and validate model outputs through real-world monitoring.

KEYWORDS: *Human health, PFAS, industrial chemicals, circular economy, exposure assessment, Bayesian updating*

1. INTRODUCTION

Knowledge of the fate and transport of persistent, mobile, and potentially toxic industrial chemicals (iPMTs), a large group of compounds to which per- and polyfluoroalkyl substances (PFAS) belong, is limited but growing. The study of PFAS in the last decades has grown exponentially: while only 595 instances of PFAS were found in the literature between 1940 and 2002, 2,500+ papers were published between 2002 and 2020, with another 2,000+ papers published between 2020 and 2024.[1] Although PFAS detection, treatment, and remediation is experiencing increased attention in the scientific community, many uncertainties remain, related to fate and transport and to the effect of PFAS on environmental and human health.

A potential way to address these uncertainties is to use risk-based exposure assessments. Risk-based methods for microbiological contaminants have been widely applied in scientific settings. In water systems, the acute risk of microbiological contaminants is usually assessed via quantitative microbial risk assessment (QMRA). The principle of QMRA was adopted from risk assessment in the food industry, and guidelines for conducting QMRA have been published by the World Health Organization, among others.[2] Many QMRAs are conducted in a probabilistic way, which allows the variability and the uncertainty which may be inherent to a system to be assessed.[3−5] Bayesian networks are increasingly applied for probabilistically evaluating risks in environmental systems,[6−9] including microbial risk of water systems.[10−12]

For chemical contaminants in trace concentrations, the human health effects of which are often unknown but assumed to be chronic, quantitative chemical risk assessment (QCRA) has begun to be investigated in research settings.[13−15] Existing exposure models for chemical risk assessment (e.g., the US EPA's SHEDS) provide highly detailed results and, as a result, require a large amount of input data. While this offers significant advantages for subsequent risk management, it is

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also very time-consuming. There is a need for simple and fast exposure models that can serve as early warning tools and which can be adjusted to site-specific conditions. Fate and transport models and QSAR-based approaches support exposure characterization and hazard identification but do not enable the explicit propagation of uncertainty associated with individual processes within a treatment train. Their applicability to indirect potable water reuse (IPR) systems is limited. In this context, EWEX provides a simple and very flexible contribution by explicitly representing uncertainty across sequential treatment processes within a probabilistic framework for chemical risk assessment.

With the passage of the European Green Deal in 2020, greater focus has been placed on sustainable reuse of materials and the transition from a linear to a circular economy. However, the lack of knowledge of the chemical fate in circular economy routes presents a hurdle to achieving circularity. Indirect potable water reuse, when treated wastewater is introduced into an environmental buffer (e.g., reservoirs, aquifers) before being abstracted for drinking water production, is one such route with limited knowledge. Probabilistic assessment of chemical risk in drinking water,[15] as well as the risk of chemical mixtures,[14] has been a recent topic of study, with the relative potency factor (RPF) approach developed for PFAS[16] applied to compare mixture risk in bottled and tap water.[14] However, the low concentrations and analytical detection limits for PFAS and other compounds in drinking water complicate quantitative risk assessment. The difficulty of dealing with left-censored data[17] or potentially greater concentrations of PFAS in effluent than in influent (e.g., negative removal due to precursor transformation products), as is often seen during conventional municipal wastewater treatment,[18] is still a topic of discussion in chemical risk assessment.

Chemical exposure assessments could serve as an early warning system for drinking water companies so that they are prepared for particular compounds or scenarios ahead of time.[19] Many benefits to developing a probabilistic early warning system exist. Such a system would prevent risk assessment tools from being unnecessarily conservative for the general population and from underestimating the effect on susceptible populations.[20] To allow information across different spatial and temporal timelines to be used, Bayesian models can be used to produce credible, local estimates where monitoring is sparse and to propagate climate or management scenario uncertainty into risk forecasts, all of which are useful for planning and adaptive management.[21] Biomonitoring data and toxicokinetic/dynamic modeling, which is especially useful for many low-concentration chemicals,[22] can also be integrated. Probabilistic results can be directly referenced for management decisions, as Bayesian methods make trade-offs and confidence explicit for policy makers.[23]

A tool or model providing actionable results, such as which compound out of many evaluated should be prioritized for remediation first or what effects different scenarios would have on the exposure to the compound, is missing. Particularly for industrial chemicals and PFAS, an integrated risk assessment approach would help their producers develop strategies to manage and mitigate risks to surface water and groundwater.[24] This study therefore presents the first application of Bayesian updating to assess the exposure to human health from PFAS and iPMTs in indirect potable water reuse (IPR).

2. METHODS

This paper explains how the probabilistic early warning exposure assessment (EWEX) model developed in the EU Horizon 2020 PROMISCES project can quantify exposure risks from persistent and mobile compounds. The model estimates contaminant concentrations in the final water matrix based on the cumulative effects of treatment processes and dilution and evaluates health or environmental risks by comparing these concentrations against compound-specific reference values. The full methodological framework, including model structure, assumptions, and equations, is described in detail in PROMISCES Deliverable D2.5.[25] The present paper demonstrates the EWEX approach using the example of the IPR cycle, composed of conventional municipal wastewater treatment, surface water dilution, bank filtration, and drinking water treatment.

2.1. Removal Factor Approach

The EWEX model simulates the concentration profile of individual compounds along a predefined treatment and an environmental pathway. Each treatment step is characterized by a removal factor (RF), representing the proportion of a compound removed. These RFs are treated probabilistically and informed by a combination of the following: a) literature data (median or mean values from individual studies); b) site-specific experimental data; and c) model-based estimates, if applicable.

2.1.1. Bayesian Updating of Removal Factors. A central feature of the EWEX model is its Bayesian updating approach, which addresses the epistemic uncertainty common in removal efficiency data for persistent and mobile compounds such as PFAS and iPMTs. Rather than relying on deterministic removal factors, the model treats the removal factor of each process step as a probability distribution, reflecting varying levels of knowledge and data availability.

2.1.2. Prior Distributions. A prior distribution is applied for the RF of each treatment process to reflect the default assumption before incorporating empirical data. Instead of using a noninformative uniform distribution, a convex-shaped beta distribution is used as the prior, due to its symmetric shape, with alpha and beta parameters both set below 1, and its capability to assign higher likelihood to extreme outcomes (e.g., complete removal or no removal), which supports a precautionary risk assessment. In a uniform distribution between 0% and 100% removal, the probability of a worst-case removal being $\leq$ 1% is only 1%. Therefore, from a risk-based perspective, the worst case cannot be adequately covered, especially with several processes in series. A beta distribution ensures that worst-case scenarios are inherently considered in the absence of substantial evidence (see Figure 2). A detailed explanation of the selection of the prior distribution, as well as a comparison of the beta distribution with other possible prior distributions, can be found in the SI.

2.1.3. Likelihood Functions from Data. The prior distribution is then updated using the data available. If literature data is available, a representative RF (typically the mean or median reported removal as a rounded integer) is extracted from each reported treatment site and incorporated into the likelihood function. To avoid overconfidence of high removal factors from sparse literature, a conservative adjustment is applied as an additional removal factor (RF_0) (eq 1):

$$RF_0 = \frac{0.1\% + \sum_{i=0}^{n} RF_i}{n+1} \quad (1)$$

RF_0 depends on the removal factors from the literature (RF_i) and the number of sites included (n). The normally distributed likelihood function is then created by literature removal factors and RF_0, which is treated as a literature value.

When few literature values are available, RF_0 shifts the normal distribution to the left, toward lower removal factors. The more literature values that are available, the more negligible the effect of RF_0 becomes. The calculation of RF_0 also ensures that even a single literature value is sufficient to create a normal distribution. Using a coefficient of '0.1%' instead of '0%' in eq 1 enables the calculation of the mean and standard deviation, even when the literature values are 0%.

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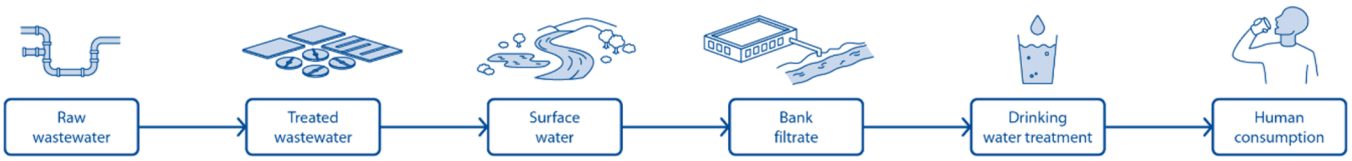


Figure 1. Modeled IPR route (Reprinted or adapted with permission under a Creative Commons Attribution 4.0 International license from 10.5281/zenodo.15308552. Copyright 2025 Zenodo).

If site-specific data are available, all measured RFs are included (rounded as integers) without aggregation, as site-specific data are considered the most representative. The conservative adjustment is done in the same way as that for literature data. In this case, literature values can be omitted if they are deemed to be insufficient for describing the site-specific process. If modeled data, such as from process-specific models, are available, these outputs can also be used to update the prior, but their influence is limited to prevent dominance over empirical evidence. For processes associated with a removal range, or where the concentration of the compound is reduced due to an applied treatment, removal percentages were initially gathered from the literature and later from experimental results from the PROMISCES project.

2.1.4. Posterior Distribution and Propagation through the Exposure Route. Using Bayes' Theorem (eq 2), the prior distribution $P(A)$ is combined with the likelihood function derived from available data $P(B|A)$, as well as the marginal probability $P(B)$, to produce a posterior distribution for the removal factor $P(A|B)$.

$$P(A|B) = \frac{P(B|A) \times P(A)}{P(B)} \quad (2)$$

Each treatment process in the exposure route uses the posterior removal factor distribution to simulate the contaminant attenuation. Output concentrations from each process serve as the input for the next step, allowing uncertainty to propagate through the entire exposure route. If on-site data are available, then the removal factors drawn from the posterior distribution are randomly applied to the input concentration. Otherwise, the lowest removal factors are applied to the highest input concentration and vice versa to account for potential site-specific differences compared with literature data. Final concentrations are expressed as percentile distributions, reflecting the cumulative uncertainty from all upstream processes.

2.2. Dilution and Contamination Processes

At a site, the dilution or contamination process depends heavily on local conditions. In addition to the proportion of receiving water, background concentrations significantly influence contaminant concentrations. For this reason, unlike for removal processes, it is not possible to use prior assumptions or literature values in the EWEX tool. The EWEX tool describes the concentration following a mixing process according to eq 3.

$$c_{out} = c_{in}(1 - x_w) + c_w x_w \quad (3)$$

In this equation, x_w is the proportion (between 0 and 1) of the receiving water, and c_w is the background concentration in the receiving water. Both values were drawn from a predefined normal distribution. Unlike technical removal processes, mixing processes are often highly dynamic and are dependent on environmental conditions. However, the EWEX model is static and represents only the average values. To account for different mixing conditions (e.g., due to seasonality, climate change, or specific events) in the assessment, multiple exposure scenarios with different mixing characteristics were defined.

2.3. Exposure Route

The model was used to model the IPR route, as depicted in Figure 1. For treated wastewater, conventional municipal primary and secondary treatments were assumed. For drinking water treatment, aeration, granular activated carbon (GAC), and ion exchange resins (IX) were assumed. Furthermore, two dilution steps of wastewater treatment plant effluent by surface water and of bank filtrate by groundwater were integrated. Surface water and groundwater were assumed to be uncontaminated (e.g., 0 ng/L concentration). In the here presented IPR exposure route, the proportions of the diluting water after dilution are described as a normal distribution with a mean value and standard deviation. These were 0.66 and 0.2 for surface water, which can be considered a low dilution by surface water,[26] and 0.25 and 0.2 for groundwater, which can be considered a typical ratio of bank filtrate at high-intensity bank filtration sites. The dilution factor and background concentration are highly site specific and cannot be transferred to other regions.

2.4. Removal Data

The functionality of the EWEX approach is demonstrated in this paper using 3 compounds: PFOS, trifluoromethanesulfonic acid (TFMSA), and carbamazepine (CBZ). For PFOS, a large number of removal data for individual processes were available. For TFMSA, there is a lack of literature data. For CBZ, only a small amount of literature data was collected, as it was not the focus of the PROMISCES project. The CBZ example was nevertheless included as it shows how meaningful results can be obtained even without extensive literature research. Furthermore, the model evaluated 14 compounds to show how the EWEX can be used for substance screening in different scenarios. While literature data was scarce for most of the PFAS, experimental results from lab-scale GAC rapid small-scale column tests with bed volumes between 10,000 and 20,000 were used for both assessments to account for short-chain PFAS removal.[27] These column tests and the experiments with IX were conducted with tap water spiked with PFAS and iPMTs, which added additional uncertainty to the assessment and results. Literature data used for the demonstration and screening case are provided in the Supporting Information.

2.5. Starting Concentration and Risk Characterization

To assess the potential human health risk, final modeled concentrations were divided by compound-specific reference values to calculate reference quotients (RQ). A compound was considered of concern when the RQ exceeded 1, indicating a potential to surpass health-based exposure thresholds. However, legal threshold values are not defined for each individual PFAS compound, and PFAS toxicity data are constantly being updated. The EU Drinking Water Directive (2020/2184) provides guideline values for the sum of 20 PFAS (100 ng/L).[28] To derive threshold values for individual compounds, relative potency factors (RPFs), which compare the toxicity of a specific PFAS compound to that of PFOA, were used. First, the threshold value for PFAS-20 was divided by the RPF of each compound. This gives the maximum tolerable concentration of a single PFAS compound from a toxicity perspective, assuming that no other PFAS from the PFAS-20 group are present. For PFOA, this value was exactly 100 ng/L. For PFNA, which is estimated to be ten times more relevant to human health, the value is only 10 ng/L. These maximum values were then divided by 20 to indicate the tolerable concentration of a single PFAS compound, assuming that all the compounds equally contribute to overall toxicity. The RPFs and corresponding reference values[16,29] are listed in Table 1. Using RPFs allows the EWEX model to incorporate in vivo end points for individual PFAS compounds and to include additional compounds not covered by the PFAS-20 sum specified in the Drinking Water Directive. While RPF-derived reference values are suited for the initial screening of priority compounds, more in-depth evaluations should

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Table 1. RPF, Reference Value, and Starting Concentration of Compounds Assessed

Compound	RPF	Reference value [ng/L]	Demonstration case concentration − 3 compounds [ng/L]	Screening case concentration − 14 compounds GAC vs IX [ng/L]
PFBA	0.05	100	-	19
PFPeA	0.05	100	-	27
PFHxA	0.01	500	-	270
PFHpA	1	5	-	58
PFOA	1	5	-	550
PFNA	10	0.5	-	20
PFDA	10	0.5	-	27
PFBS	0.001	5000	-	37
PFPeS	0.6	8.3	-	830
PFHxS	0.6	8.3	-	54
PFOS	2	2.5	50	449
TFMSA[a]	-	1	20	100
Benzotriazole	-	3000	-	44000
Carbamazepine	-	300	6000	5000

[a]Relative Reference Value and Starting Concentrations, Dimensionless.

use toxicologically derived threshold values for individual compounds, if available.

The reference values for CBZ and benzotriazole were obtained from the German Environment Agency's list of health-based guidance values as of 2023.[30] No reference value was available for TFMSA. However, the EWEX model can evaluate substances without reference values, which is essential for substances that have received little attention to date. This is achieved by assuming a reference value of 1 and entering the initial concentration as a multiple of that value. The model then evaluates the removability of the substance along the exposure path.

To demonstrate the EWEX model on PFOS, TFMSA, and CBZ, the initial concentrations (demonstration case concentration) were set at 20 times the reference value of each compound to ensure comparability. In contrast to this demonstration case, the initial concentration of the screening case is mostly based on literature values of studies sampling raw wastewater. The concentrations used for calculation were set as either the database maximum or the 100-fold of the compound's reference value for TFMSA and PFPeS, a very conservative assumption. A database containing all published values for the concentrations of these substances in raw wastewater is provided in the Supporting Information. Model outputs are presented as spider plots with colored percentile distributions to capture the probabilistic range of exposure under different conditions.

3. RESULTS AND DISCUSSION

The functionality of the EWEX approach is demonstrated using PFOS, TFMSA, and CBZ. Their exposure calculations vary considerably because of differences in the underlying data basis. In addition, the two exposure pathways, which differ in their final drinking water treatment step, were compared for 14 substances, and the results were interpreted. To demonstrate the possibility of using the EWEX for backward calculation, a

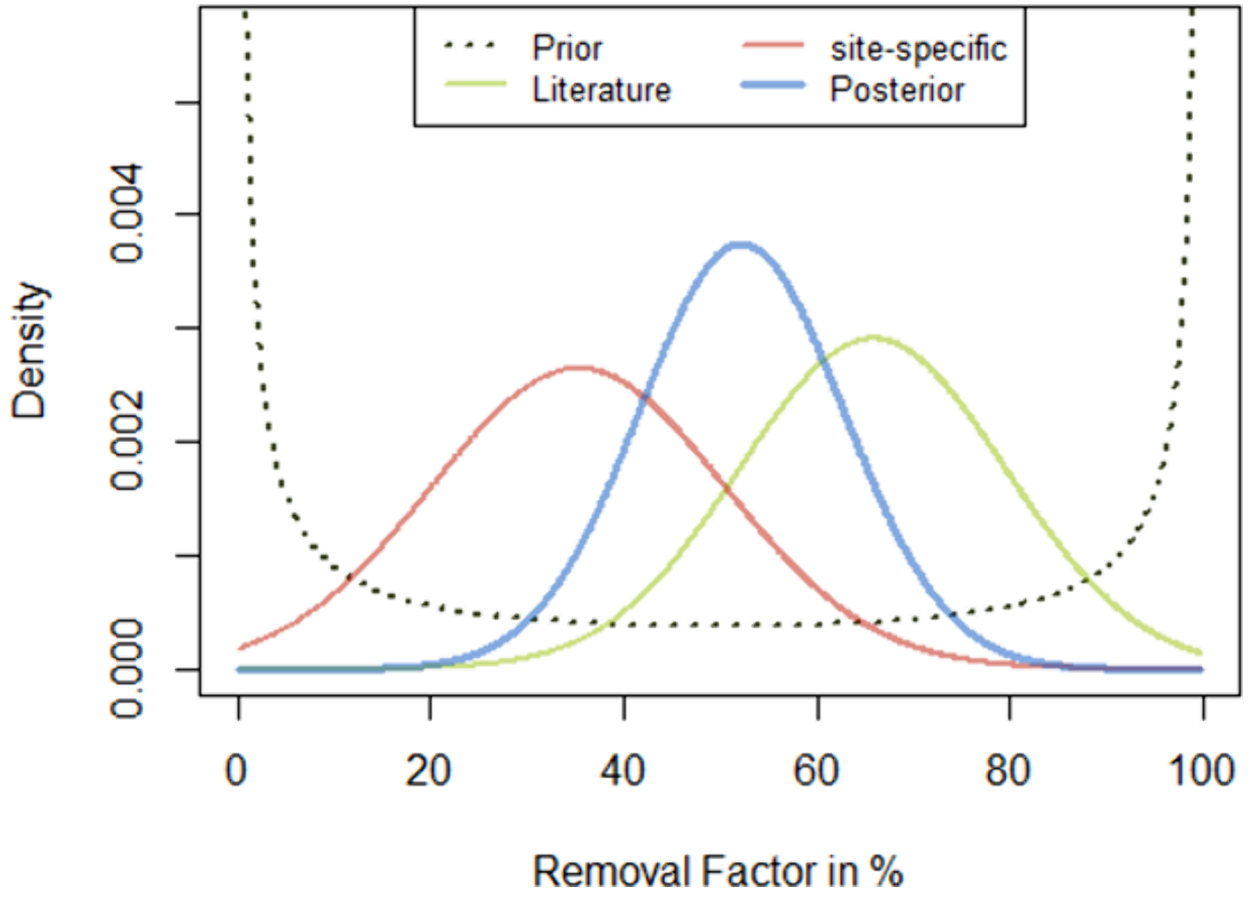


Figure 2. Prior distribution (dotted), literature likelihood distribution (green), measurements likelihood distribution (red), and posterior distribution (blue) of removal factors for PFOS by GAC.

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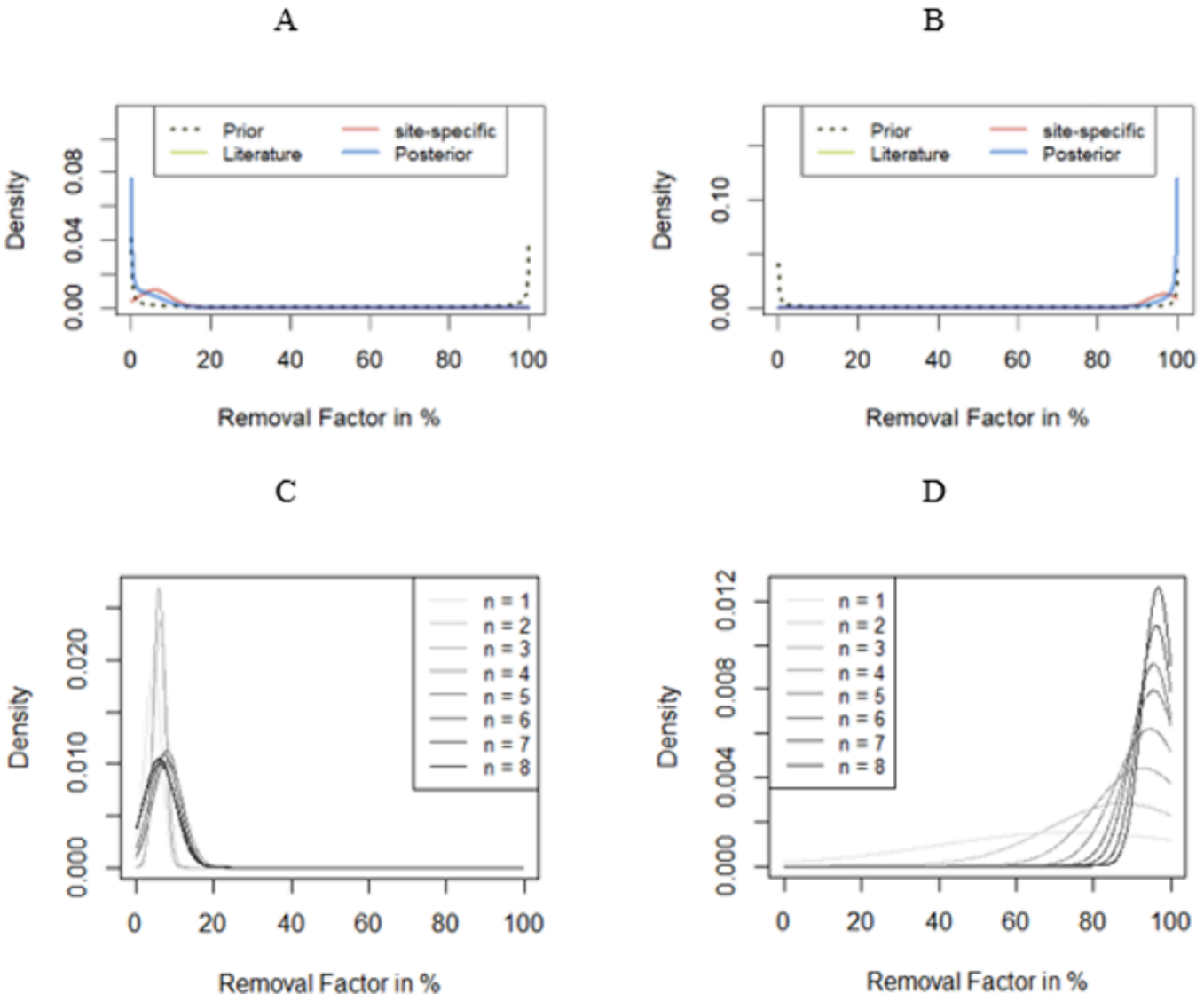


Figure 3. Prior distribution, likelihood, and posterior distribution of TFMSA (A) and CBZ (B) removal by GAC in drinking water and the shape of the likelihood distribution with increasing number of measurements for TFMSA (C) and CBZ (D) removal.

tolerable starting concentration was determined for PFOA, based on the final reference value and the GAC exposure route.

3.1. The Impact of Available Data on the Removal Factor Distribution

In the exposure route, GAC is used as the final step in drinking water treatment. For PFOS, there were six values for GAC removal in the database (90%, 76%, 56%, 49%, 68%, 64%). In on-site column tests, removal performance was slightly worse, with removal factors of 33%, 27%, 28%, 42%, 18%, 69%, and 34%. Figure 2 shows the relationships between the prior, literature data, measurement data, and posterior distributions for PFOS. The prior distribution is clearly symmetrical, reaching its maximums at 0% and 100% removal. Without further data, this distribution would be adopted by the posterior. For PFOS, however, the posterior is dominated by the likelihoods based on the literature and measurement data. All available information leads to the assumption that PFOS can be removed moderately well by GAC. There are many possible reasons why removal efficiency may differ between literature data and a specific system. Local conditions, such as the water matrix or operational treatment conditions, can have a significant impact. For literature values, systems operating under "standard conditions" were selected, in which, for example, GAC filters are operated with economically reasonable bed volumes. In a case study, however, a GAC filter may be designed to remove a specific substance as effectively as possible, which may involve operation at a lower bed volume. If measured values are more realistic for on-site than literature values, literature values can be disabled in the calculation. In this case, the water matrix obtained from the column experiments is specific to the site and therefore supports the use of only site-specific data. However, as these were lab-scale experiments, literature values were also used.

The database did not contain any removal values for TFMSA or CBZ by GAC. While for TFMSA no values were found in literature, no exhaustive literature review was conducted for CBZ. In the on-site column tests, TFMSA was poorly removed (6%, 8%, 5%, 15%, 7%, 3%, −3%, 4%), while CBZ was well removed (99%, 98%, 99%, 98%, 97%, 94%, 99%, 99%). Figure 3A and Figure 3B show the resulting distribution functions for the removal of both compounds: the posterior distribution for TFMSA shows that a high removal

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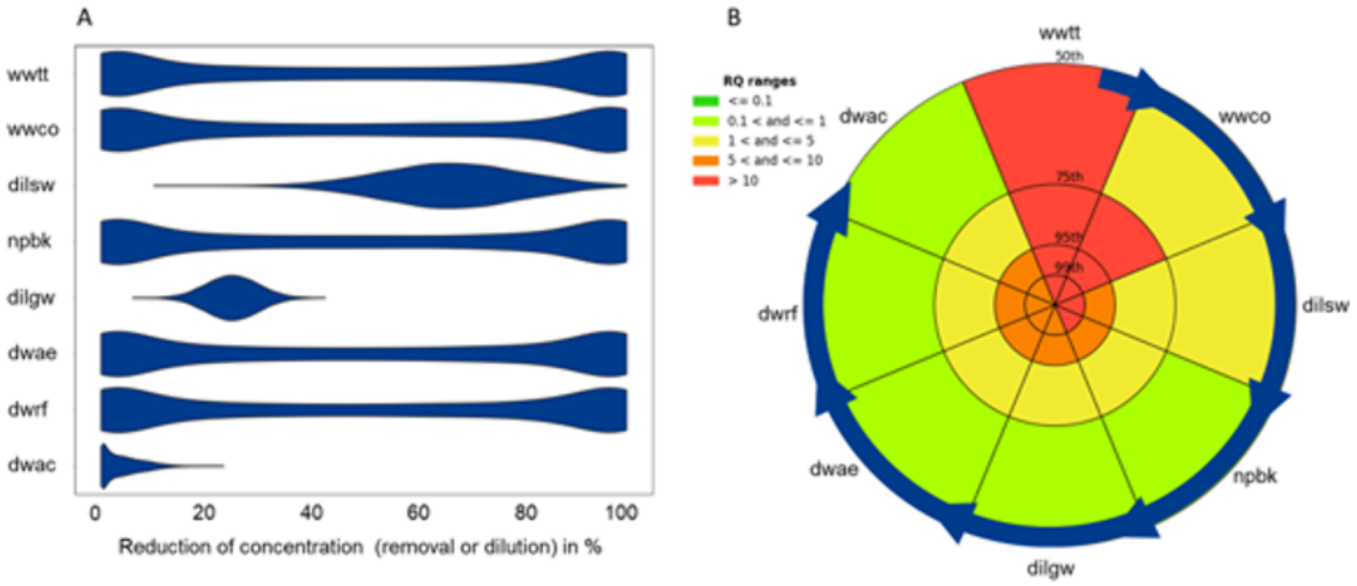


Figure 4. Posterior distributions of removal factors (A) and final reference quotient percentiles (B) for TFMSA along the treatment train. In dilution processes, the removal factor is calculated based on the decrease in concentration. (wwtt: primary and secondary wastewater treatment, wwco: coagulation, dilsw: dilution by surface water, npbk: bank filtration, dilgw: dilution by groundwater, dwae: aeration, dwrf: rapid filtration, dwac: activated carbon treatment).

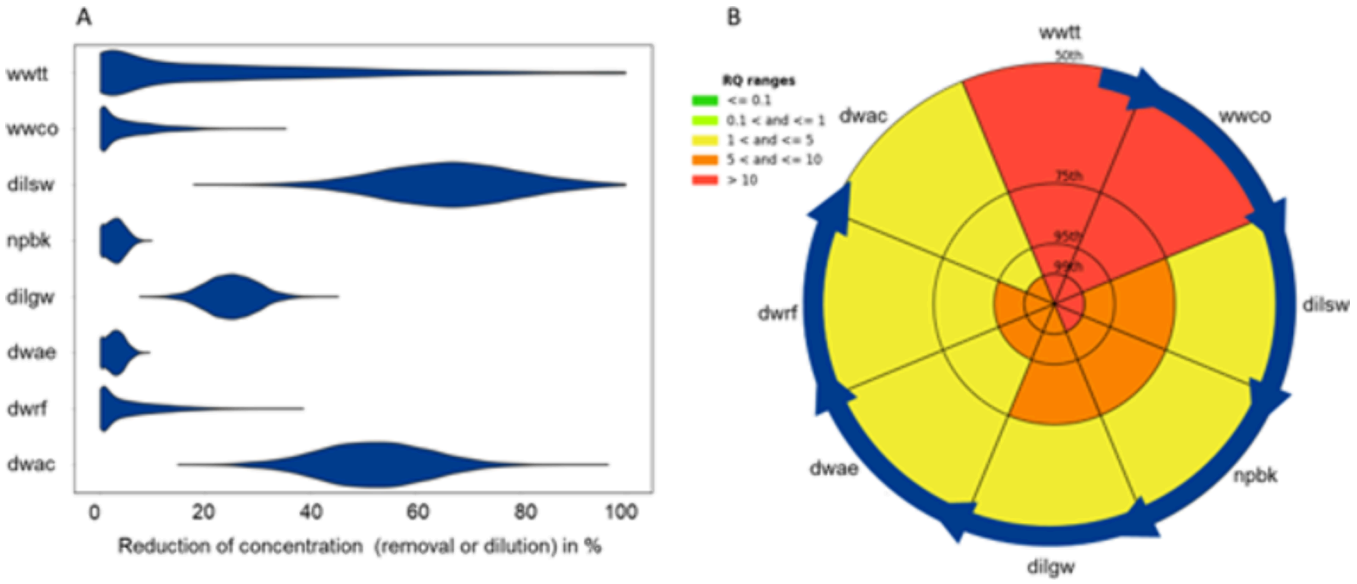


Figure 5. Posterior distributions of removal factors (A) and final reference quotient percentiles (B) for PFOS along the treatment train. In dilution processes, the removal factor is calculated based on the decrease in concentration. (wwtt: primary and secondary wastewater treatment, wwco: coagulation, dilsw: dilution by surface water, npbk: bank filtration, dilgw: dilution by groundwater, dwae: aeration, dwrf: rapid filtration, dwac: activated carbon treatment).

rate is nearly impossible, whereas for CBZ, it is the other way around. If the probability function is not created with all eight measured values, but rather updated step by step with the measured values, the impact of the conservative adjustment becomes apparent. For TFMSA, even a single measurement value with low removal performance results in a fairly narrow probability distribution close to 0% (Figure 3C). Including additional similar measurement values does not notably change the distribution. From n = 4 onward, when the relatively "high" 15% removal rate is included in the calculation, the distribution becomes slightly wider.

For CBZ, a single measured high removal rate leads to a broad distribution. Combining this broad distribution with the prior leads to a posterior distribution that has its maximum at high removal values. However, there is still a notable probability of low removal factors. The more measurements of similarly high removal are included, the narrower the probability distribution becomes and shifts toward 100%. The conservative adjustment thus ensures that high removal values must be confirmed multiple times before they are considered to be reliable enough.This demonstrates how the EWEX model integrates uncertainty into exposure calculation in a risk-based manner.

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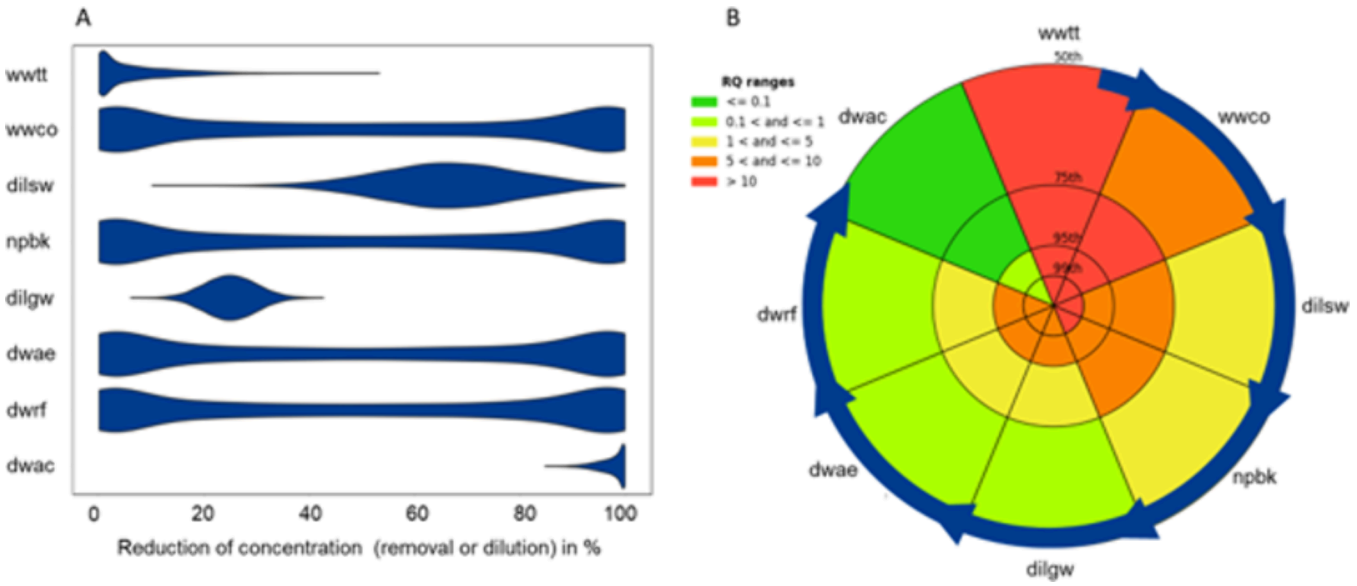


Figure 6. Posterior distributions of removal factors (A) and final reference quotient percentiles (B) for CBZ along the treatment train. In dilution processes, the removal factor is calculated based on the decrease in concentration. (wwtt: primary and secondary wastewater treatment, wwco: coagulation, dilsw: dilution by surface water, npbk: bank filtration, dilgw: dilution by groundwater, dwae: aeration, dwrf: rapid filtration, dwac: activated carbon treatment).

3.2. The Impact of Available Data on a Treatment Train Level

Figure 4, Figure 5, and Figure 6 show the RFs and RQs after each process in the treatment train. On the left-hand side (A), violin plots show RF distributions per treatment step or the concentration reduction due to dilution. On the right-hand side (B), spider plots show the 50th, 75th, 95th, and 99th percentiles of the RQ distribution after each treatment step.

The TFMSA concentration is assumed to be 20 times the reference value at the beginning of the exposure pathway. No literature data or measurement data were available for conventional wastewater treatment (wwtt) or coagulation (wwco). This can be seen from the RF distributions, which have their maximum values at 0% and 100% and correspond directly to the prior (Figure 4). In the spider plot (Figure 4B), both processes influence the 50th percentile of the concentration, while the higher percentiles remain in RQ > 10. Without available data, a large portion of the concentration distribution remained unchanged after the process. This is again observed after the coagulation process and is possible only because the RFs are not randomly combined with the input concentration. This ensures that an exposure route of prior-driven processes cannot significantly improve the exposure assessment results. Further along the exposure route, dilution with pure surface water and groundwater occurs. Both dilution processes lead to a notable concentration reduction and, thus, to an improvement in the exposure assessment (as seen in the spider plot). However, the subsequent bank filtration, aeration, and rapid filtration steps do not lead to any further concentration reduction as they are also described exclusively by the prior. Measured values were available again for final GAC treatment. However, only a small amount of TFMSA was removed, and it also does not lead to an improvement in the exposure assessment. At the end of the exposure pathway, the 75th percentile of the RQ is between 1 and 5, and the 95th and 99th percentiles are between 5 and 10. A concentration above the reference value cannot be excluded. The dilution effect alone is therefore insufficient to ensure that the reference value is met at the end of the exposure route. In this case, either additional data or further treatment steps with known removal efficiencies are required to bring the 75th percentile of the RQ down below 1.

In contrast to TFMSA, a large amount of literature data on PFOS removal in various treatment steps was available. For primary and secondary wastewater treatment, some values varied, but most described poor removal. A similar picture emerged for the subsequent coagulation process, although the literature values were slightly more uniform. This narrows the posterior distribution and makes high removal factors unlikely. The PFOS concentration distribution after these processes can be directly compared to the TFMSA distribution, as initial concentrations for both compounds were 20 times their reference values. For PFOS, all RQ percentiles after the first two processes were >10. This means that exceeding the PFOS reference value after the first two processes is more critical than for TFMSA, which is logical since PFOS is known to be difficult to remove, and therefore, based on current knowledge, exceeding the reference value is more likely. Similar to TFMSA, dilution processes lead to the greatest improvement in assessment results. Although PFOS can be more effectively removed with GAC than with TFMSA, this removal performance does not notably improve the result. As with TFMSA, the assessment at the end of the exposure pathway is critical. The key issue here is not the lack of knowledge but rather the poor removal performance reported in the literature. If on-site processes could work better than those reported in the literature, including more on-site data could lead to a more realistic result. Otherwise, further treatment steps are necessary to further reduce the RQ of all percentiles.

Removal of CBZ in many water-treatment steps has been well described. However, CBZ was not the focus of the project; therefore, a comprehensive literature search for its removal was not conducted. Consequently, many posterior distributions for CBZ resemble those of TFMSA for which no data are available. There are two differences, however: First, the

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removal performance of the conventional wastewater treatment was considered. Second, unlike TFMSA, CBZ could be effectively removed in activated carbon column experiments. Despite the limited data collection, the removal performance combined with dilution processes means that even the 99th percentile is below the reference value. In this case, no further measures need to be taken as the limited information is sufficient. This reduces the workload and time, which can be used for the risk management of more critical compounds.

This demonstration shows that both situations - lack of knowledge and poor removal performance - are critically evaluated by the EWEX model. Conservative prior distributions and Bayesian updating provide a precautionary risk estimation framework, favoring overestimation of risk in the absence of robust removal evidence (as seen for TFMSA). On the other hand, the pragmatic approach does not necessarily require comprehensive data collection to be able to exclude elevated exposure (as seen for CBZ).

3.3. Substance Screening of Two Scenarios Using GAC and IX Exposure Routes

EWEX is a risk-based early warning tool which produces results regardless of data basis. Depending on the available data, there are three possible interpretations of the results.

1. **The result is dominated by knowledge gaps**. In this case, no real concentration is simulated. Because of the prior and the conservative starting point, the result will generally indicate an elevated risk. However, in some cases, even one well-studied process may be sufficient to rule out an increased risk.
2. **The result is dominated by literature values**. Again, no real concentration is simulated in this case. Average values from the literature allow for reliable general substance screening and comparison of exposure pathways. However, the on-site situation can be very different, especially when literature values greatly vary.
3. **The result is dominated by on-site measurements**. The model is adapted to local conditions. The actual pollutant concentration at the case study site is calculated, and the model can be validated. Different future scenarios can be calculated by changing the treatment steps or hydrological conditions.

This screening primarily involves the first two cases and does not provide an accurate on-site assessment. Nevertheless, the screening demonstrates how priority substances can be identified and how they vary among different scenarios. In the GAC treatment exposure route (Figure 8A), the highest risks found were for PFOS and PFOA, followed by TFMSA, PFPeS, PFNA, and PFDA. The percentile at which the RQ is exceeded can be quickly identified when visualizing RQ values as a color-coded spider plot of distribution percentiles. Results showed that PFOS consistently exceeded reference values across multiple percentiles, even after treatment, indicating a high level of concern. Although short-chain PFAS such as PFBA and PFBS cannot be effectively removed in wastewater[31] or drinking water treatment,[32] no increased risk has been identified for these compounds.

Figure 7 shows a comparison of the EWEX removal factors for PFBA (negligible risk) and PFOA (increased risk). In primary and secondary wastewater treatment processes, as well as in rapid filtration and activated carbon filtration, PFBA is removed less effectively than PFOA, which is consistent with drinking water treatment results.[32] No PFBA removal data

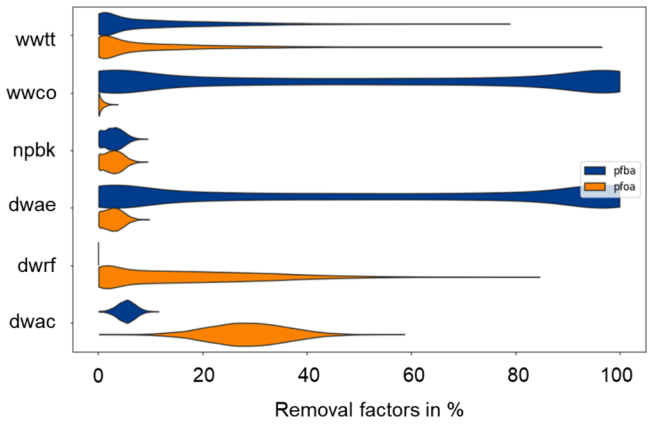


Figure 7. Comparison of PFBA (blue) and PFOA (orange) removal factors in the GAC scenario (wwtt: primary and secondary wastewater treatment, wwco: coagulation, npbk: bank filtration, dwae: aeration, dwrf: rapid filtration, dwac: activated carbon treatment).

were available for the other processes. As with any risk assessment, the outcome depends significantly on the initial concentration and threshold value used. The assumed initial concentration of PFBA was 19 ng/L, which is below the reference value of 100 ng/L. A high reference value of 100 ng/L was used because the RPF of PFBA is low at 0.05[33] compared with that of PFOA. For PFBA, the combined overall low amount of information, on both input concentration (source strength) as well as removal efficiency (treatment performance), led to no increased risk for PFBA in this assessment. However, this result would change with different input concentrations or newer toxicological findings influencing the reference value. Additionally, it is possible that PFBA concentrations in wastewater could increase in the future due to ongoing production and high persistence, whereas PFOA has been restricted in many countries.[34]

The spider plots allow for a rapid compoundwise comparison of the two scenarios. IX generally showed better PFAS removal; however, this was insufficient to lower all percentiles of the RQ distribution below 1. In contrast, the two non-PFAS compounds, CBZ and benzotriazole, were poorly removed. Although there was no risk of exceeding the threshold observed in the GAC exposure route for both compounds, exchanging the final treatment step resulted in an RQ greater than 1, even for the 75th percentile of the distribution. This shows how the average concentration of pollutants can decrease, yet more compounds are classified as critical. Replacing GAC with IX could lead to a less critical situation if there were greater dilution by surface or groundwater or if the initial concentration was lower. This demonstrates the importance of evaluating processes in the context of an overall scenario and objective.

Since the starting concentration of the compounds was based on worst-case literature assumptions, accurately measuring the initial concentration is crucial to obtaining a more realistic estimation of the risk. If the threshold value is still exceeded in both cases, then individual treatment steps can be optimized to improve the removal performance of problematic substances (e.g., increasing the bed volume in the GAC filter). Alternatively, both processes (GAC and IX) could be combined into a single exposure route, or additional processes can be added. Furthermore, a closer analysis of the distribution of removal factors can provide information about

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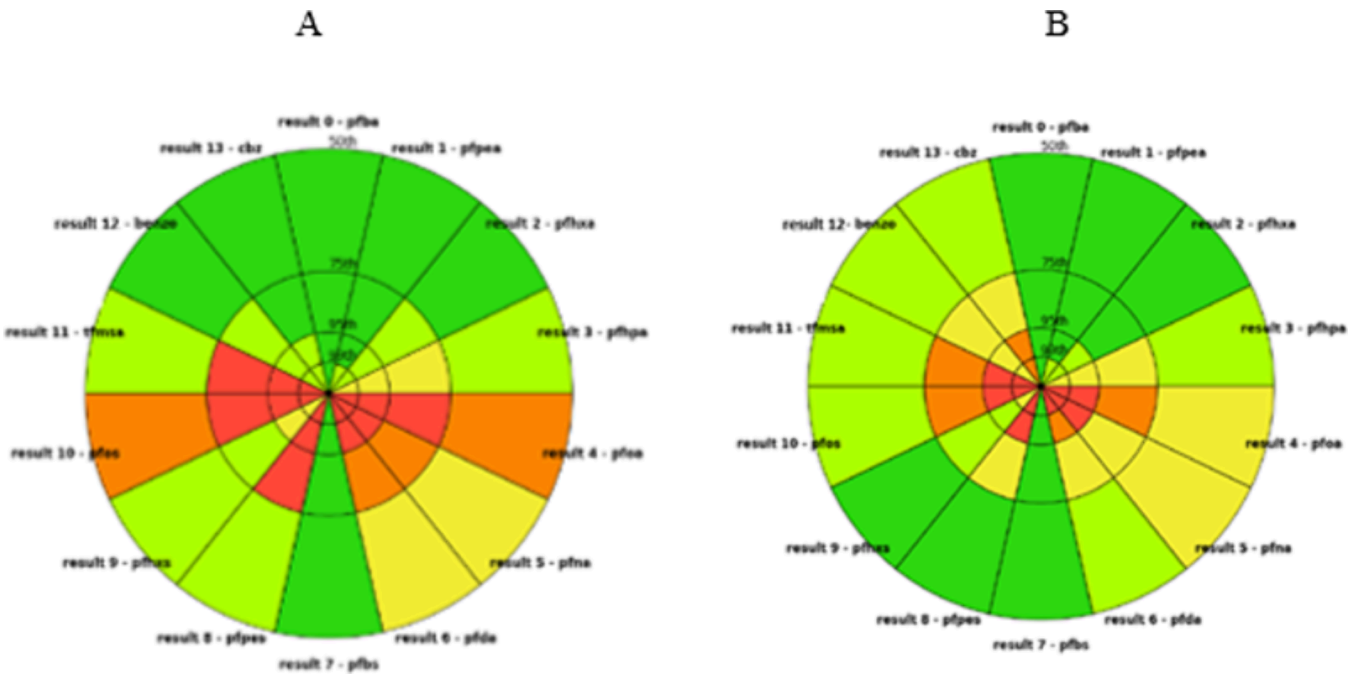


Figure 8. Spider plot of the scenarios with a) GAC and b) IX as final drinking water treatment. (Reprinted or adapted with permission under a Creative Commons Attribution 4.0 International license from 10.5281/zenodo.15308552. Copyright 2025 Zenodo).

which processes have the most significant knowledge gaps as well as where it is important to close these gaps with regard to problematic substances.

3.4. Estimating the Tolerable Starting Concentration

Under the assumptions taken, none of the compounds were compliant with their reference values, largely due to conservative estimates of raw wastewater concentrations, which were set as either the database maximum or the 100-fold of the compound's reference value, due to lack of on-site data. To address this, the model can estimate the maximum tolerable starting concentration: the inlet concentration below which even the 99th percentile of the RQ distribution remains below 1, indicating compliance across (practically) all modeled outcomes. This is determined by iteratively adjusting the input concentration until all percentiles in the output fall below risk thresholds: for PFOA, this threshold was found to be 15 ng/L. Similar analyses for other priority compounds enable direct comparison of measured concentrations to tolerable benchmarks, supporting risk assessment even when data are limited. Even for compounds which do not have defined reference values, the model can provide a tolerable multiple of an assumed reference value, allowing relative risk evaluation despite regulatory data gaps. In this way, the EWEX model can support meaningful risk contextualization and management, even for poorly characterized compounds and treatment processes.

4. CONCLUSION

This study demonstrates the application of a Bayesian probabilistic EWEX model to evaluate contaminant risks in the IPR. By incorporating both literature-derived and site-specific data, the EWEX model provides a flexible framework capable of addressing data uncertainty, which is a key barrier in assessing emerging contaminants. Scenario analyses showed that river dilution had a strong effect on reducing compound concentrations. These results emphasize the importance of both the hydrological setting and the choice of wastewater and drinking water treatment technologies for mitigating exposure.

The model's sensitivity to data type and quality was demonstrated through the assessment of PFOS, TFMSA, and CBZ. While PFOS was informed by abundant but inconsistent literature data, TFMSA and CBZ relied on experimental results, resulting in low removal for TFMSA and high removal for CBZ, especially via GAC. These findings highlight the essential role of both experimental and literature data in improving risk prediction and stress the need for robust, transferable data sets to reduce uncertainty in PFAS exposure assessments. The study highlights the critical importance of robust monitoring data and advanced treatment technologies in ensuring drinking water safety in IPR. Particular treatment steps, such as bank filtration, are still lacking published information in terms of PFAS transport and/or removal.[35] Future research should focus on expanding the data set collected in this study, especially for poorly studied compounds, refining treatment technologies targeting short-chain PFAS and iPMTs, and validating model predictions through real-world monitoring campaigns. Additional directions worth exploring would be the integration of semi-quantitative nontarget analysis (NTA) data, which could inform which additional compounds are worth tracking in a particular scenario. This study also did not include negative removals, which should be considered in future work by carefully selecting a suitable prior distribution as well as calculation methodology.

The EWEX model holds significant potential as a decision support tool for water utilities and regulators facing challenges related to iPMTs. The developed methodology can be adapted for additional treatment technologies, exposure routes, or any other combination of local considerations. The model described in this paper is designed to give an idea of what is possible based on the current knowledge rather than to predict the final concentration with extreme accuracy. This model can,

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however, complement other approaches for investigating the final quality of water reuse treatment processes[36] as a way to further identify how changes in the final exposure could be traced back to certain situations in the exposure route.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsestwater.6c00073.

Database and sources of concentrations and removal percentages for different treatment steps for the substances described in the paper, for the screening case (XLSX)

Detailed textual and graphical explanation of why the beta distribution was chosen as a prior (PDF)

Database and sources of concentrations and removal percentages for different treatment steps for the substances described in the paper, for the demonstration case (XLSX)

Accession Codes

The code developed for this model can be accessed at https://github.com/KWB-R/ewex. The associated PROMISCES deliverable D2.5 can be found at 10.5281/zenodo.15308552. The complete database can be requested by contacting the corresponding author.

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Notes

The authors declare no competing financial interest.

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