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A Bayesian probabilistic framework for next-generation chemical risk assessment: The case of PFOA in crops irrigated with treated wastewater

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ABSTRACT

Poly- and perfluoroalkyl substances (PFAS) are persistent organic pollutants ubiquitously detected across aquatic matrices, representing a significant concern for both human health and the resilience of aquatic ecosystems. Continuously released by wastewater treatment plants, there is an urgent need to develop innovative and adaptable methodologies for their risk assessment in both retrospective and prospective ways, aiming to describe uncertainty to produce a reliable risk estimate. Current methods for quantitative health risk assessment for PFAS are mostly deterministic and case-specific, with very few studies available, primarily due to limited knowledge about fate, transport, and toxicity, as well as a lack of suitable data necessitating lab- and time-intensive pilot experiments. Here, a Bayesian network-based risk assessment approach is proposed to model health risk associated with perfluorooctanoic acid through consumption of salad irrigated with reclaimed wastewater. This method, built upon evidence from the literature and experts knowledge, accounts for health risk assessment across conventional exposure scenarios, providing a valuable decision-making and risk management tool for water utilities. Its flexibility and universality allow for application even in data-scarce environments, with robustness improving as new evidence becomes available. The proposed risk model is intended to describe the multi-barrier approach perspective, facilitating forecasting and risk mitigation throughout the supply chain, and supporting efficient water management and reuse. In conclusion, the validated model was applied to data collected during a one-year monitoring campaign at two wastewater treatment plants, revealing a low risk of PFOA exposure.

1. Introduction

Climate change, with its unpredictable patterns, rapid urbanization, and increasing water demand strongly support the application of the water reuse concept (Berbel et al., 2023). Reusing treated wastewater can help mitigate water shortages and droughts, reducing the pressure on freshwater — especially in agriculture, which is currently the main user of renewable water resources, accounting for the 72% of global water footprint (Novoa et al., 2023). However, high operation costs and investments, as well as the occurrence of contaminants of emerging concern (CECs) limit the widespread adoption of this practice (Verlicchi et al., 2023).

Among CECs, per- and polyfluoroalkyl substances (PFAS) are of particular concern due to their known endocrine-disrupting effects, with perfluorooctane sulfonate (PFOS) and perfluorooctanoic acid (PFOA) being the most ubiquitous representatives in aquatic environments (Simonetti et al., 2025b). Conventional wastewater treatments are poor efficient at removing PFAS, that remain in treated effluents, discouraging the adoption of recycling schemes as well (Pan et al., 2016; Couto et al., 2019; Simonetti et al., 2025a). Municipal wastewater treatment plants (WWTPs) typically involve primary (e.g., screening and grit removal) and secondary treatments (e.g., activated sludge or biofiltration); when water reuse is intended, advanced treatments (e.g., ultrafiltration, reverse osmosis, biological activated carbon (BAC)) are often added.

Although novel techniques have been developed for the detection and remediation of PFAS (Ateia et al., 2024; Mancini et al., 2023; O’Connor et al., 2022), their fate and behavior throughout each treatment stage remain insufficiently understood and poorly managed. This

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knowledge gap represents a critical challenge that must be addressed prior to the large-scale implementation of water reuse systems (Di Marcantonio et al., 2023). A critical feature for universal monitoring and removal of emerging contaminants is the risk assessment based on standard definitions and agreements (Yadav et al., 2021).

In this context, risk analysis is an important tool for guiding actions and selecting control strategies effective in mitigating risk along the water supply chain. However, today there is still no definitive risk assessment practices for CECs (Futran Fuhrman et al., 2015; Barton-Maclaren et al., 2022), with relatively uncoordinated guidelines and the absence of a comprehensive regulation. In this context, the main EU Regulation 2020/741 has faced criticism for not adequately addressing the risks associated with these compounds. Specifically, it lacks clear guidelines for managing CECs, raising concerns that current provisions may not sufficiently protect human and environmental health in cases of non-potable water reuse (Rizzo et al., 2018).

Risk is generally defined as the product of hazard and exposure, taking into account uncertainty (Honkela et al., 2014). A full risk-based assessment approach consists of four main steps: 1. hazard characterization, 2. exposure assessment, 3. dose–response assessment, and 4. risk characterization. Health risk assessment has drawn a lot of attention from the scientific community worldwide, with many assessments relating to drinking purpose and human health (Cantoni et al., 2021; Penserini et al., 2023). However, relatively few studies have been conducted on the applications of reclaimed wastewater (Ahmadi et al., 2025; Di Marcantonio et al., 2023), with several limitations, including poorly defined exposure pathways and environmental endpoints (Specker et al., 2025). In this context, assessing treatment efficiency and developing a quantitative understanding of exposure and dose–response scenarios are crucial. Nevertheless, a fully integrated risk assessment should not rely solely on chemicals reduction targets, as health risks associated with reuse are influenced by a range of factors throughout the treatment-to-reuse process, such as the introduction of various exposure pathway variables or additional post-treatment risk mitigation measures consistent with multi-barrier approach (Beaudequin et al., 2017; Organization, 2015).

As encouraged by water sentinel authorities, addressing the complexity of this problem requires holistic, systems-based approaches that enable a comprehensive reflection on risk (Marulanda Fraume et al., 2020; Anastas et al., 2010). In this sense, the lack of quantitative data poses a significant challenge to exposure analysis in Quantitative Chemical Risk Assessment (QCRA), limiting its applicability (Yadav and Kalkal, 2024), particularly for PFAS in WWTPs, for which data are often scarce due to infrequent sampling and/or limited field-monitoring campaigns.

A Bayesian Network (BN) is a probabilistic model used to represent uncertainty and support decision-making (Mentzel et al., 2022b; Sperotto et al., 2017). BNs are modular and can be decomposed into smaller models over subsets of variables, making them highly flexible for model construction. This modularity also allows for the integration of expert knowledge such as insights from literature or expert opinions along with empirical data during model construction. Moreover, since BNs are generative models that represent the full joint distribution over variables, they can be (partially) updated with new knowledge or data using Bayes' rule (Franco et al., 2016).

To comply with the requirements of the EU Regulation 741/2020, this study proposes a novel Bayesian network approach to model and visualize the chemical risk associated with perfluorooctanoic acid (PFOA) through the consumption of raw crop, specifically salad, irrigated with reclaimed wastewater and grown in soil. PFOA was selected as the focus of this analysis, as it is one of the most ubiquitous representatives of its class, consistent with the findings of our literature review (Simonetti et al., 2025a). PFOA is known to persist in the human body with a half-life of several years and has been detected in the serum of nearly all U.S. residents, as well as in populations worldwide (Post et al., 2012). The assessment of human health risks associated with PFAS is complicated by several factors, including: (1) a lack of clarity regarding which PFAS are relevant for potential human health risk assessments; (2) limited information on the toxicity of PFAS and human exposure; (3) most human exposures likely involve unknown mixtures of PFAS; and (4) inconsistencies in toxicity test results across different assays in animals and human observations. This final aspect makes extrapolating animal data to human relevance highly uncertain, further complicated by species-specific differences in pharmacokinetics, pharmacodynamics, and mechanisms of action (Anderson et al., 2022). Based on these considerations, single-PFAS risk assessment based on literature-defined distributions may serve as a valuable starting point. PFOA concentrations in influent and effluent waters, treatment efficiencies, reference dose (RfD), and bioaccumulation factor (BAF) were gathered from the literature and integrated with expert judgment to serve as threshold values for BN parameterization. As in the paper of Beaudequin et al. (2017), this study focuses on a canonical case scenario in which post-treatment reductions and the model's capacity to simultaneously assess multiple factors influencing health risk are tested to demonstrate its potential to enhance traditional QCRA procedures under the multiple barriers paradigm (Beaudequin et al., 2016). Starting from a theoretical background on Bayesian networks, this study includes a detailed description of the scenarios and rationale behind the selection of the chemical under study. After performing a sensitivity analysis, the model was applied and validated using real-world data collected from two Italian municipal wastewater treatment plants. In all cases, the results indicated a low health risk condition, in line with the low concentrations detected.

2. Background

2.1. Current risk assessment approaches

Current methods for assessing the human health risk of emerging contaminants, such as per- and polyfluoroalkyl substances (PFAS), often rely on the calculation of Hazard Quotients (HQs), as recommended by the U.S. Environmental Protection Agency (EPA) (Lemly, 1996; Rebelo et al., 2022; Benson, 2014). The HQ is defined as follows:

$$HQ_i = \frac{EDI_i}{RfD_i} \tag{1}$$

where EDI_i is the estimated daily intake of the individual contaminant i (e.g., PFOA) through relevant exposure pathways (e.g., ingestion of contaminated food or water), and RfD_i is an appropriate reference dose, such as acceptable daily intake (ADI) (Truhaut, 1991; Khan, 2010) for European Union, representing the maximum acceptable oral exposure to a chemical substance over a lifetime without appreciable health risk. An HQ value greater than 1 indicates potential concern for human health, prompting further investigation or risk management actions. Risk is usually considered an estimation of the likelihood that an adverse effect occurs on a target population when being exposed to a chemical. Nevertheless, the result of this calculation is a number, that cannot stand alone as a scientifically defensible characterization of human health risk (Mentzel et al., 2022b). To this end, QCRA models, typically based on Monte Carlo simulations and employed for assessing public health risks from chemicals, can incorporate uncertainties across PFAS exposure pathways, turning this number into a probability distribution (Cantoni et al., 2021). Nevertheless, QCRA approaches, which rely on numerical simulations, are fundamentally data-dependent. In the case of PFAS in WWTPs, available data are often limited and of poor quality, due to high analytical costs, the lack of standardized methods, and a still permissive regulatory framework (Rizzo et al., 2018; Menger et al., 2021; Thompson et al., 2024). As a result, characterizing exposure in real-world scenarios becomes challenging, and overall risk evaluation remains inadequate in the presence of significant data gaps. In this context, BNs can integrate the QCRA framework, by addressing the difficulties in modeling exposure pathways, compensating for data scarcity, and explicitly characterizing uncertainties to produce more reliable risk estimates. Notably, QCRA outputs can serve as inputs to BN models, while BNs can be used to augment a QCRA, including expressing an entire stochastic QCRA model, using the same mathematical relationships, but implemented in a network which includes the joint distribution of all variables (Beaudequin et al., 2016; Chen and Pollino, 2012; Straub, 2009; Greiner et al., 2013).

2.2. Bayesian network: basic principles

Bayesian Networks are graphical models that represent the joint probability distribution over a set of variables. Each model consists of a Directed Acyclic Graph (DAG), where nodes represent variables and edges capture the dependencies between the variables. The joint distribution is expressed in a factorized form, where each variable is associated with a conditional probability distribution given its parent variables in the DAG. Formally, given a BN with DAG $G = (V, E)$ over variables V with edges E, the BN represents the joint distribution $P(V)$ over V as:

$$P(V) = \prod_{i=1}^{|V|} P(V_i|\mathrm{Pa}_G(V_i)) \tag{2}$$

Here, $\mathrm{Pa}_G(V_i)$ represents the set of parents of V_i in G, and $P(V_i|\mathrm{Pa}_G(V_i))$ represents the conditional distribution of the variable V_i given its parents. $|V|$ denotes the total number of variables in the model.

By exploiting this modular factorized representation, BNs allow efficient computation of posterior distributions on any subset of variables under any given observations. This modularity also help in incorporating data from various sources on subsets of variables in the BN. This capability enables uncertainty quantification and supports more informed decision-making (Pearl, 2014). BNs have been widely applied to domains where uncertainty quantification as well as expert knowledge integration is critical, such as, modeling microbial health risk (Beaudequin et al., 2017; Massiot et al., 2023; Kammoun et al., 2023; Zhiteneva et al., 2021; Bouwknegt et al., 2014) or environmental risk (Mentzel et al., 2022b; Yu and Zhang, 2021; Hokstad et al., 2006; Forio et al., 2015; Mentzel et al., 2022a; Li et al., 2018). Many software tools are available for constructing and performing inference on these models (Almond and Zapata-Rivera, 2019), including open-source libraries such as pgmpy (Ankan and Textor, 2024), bnlearn (Scutari, 2010), pyAgrum (Ducamp et al., 2020), as well as proprietary tools such as Netica and GeNIe. These tools provide functionalities for learning BNs from data and performing inference to compute posterior distributions under observed evidence.

3. Outline

As shown in Fig. 1, a BN was developed following a QCRA approach to evaluate the risk associated with waterborne PFOA, one of the most representative PFAS found in wastewater matrices. In this context, the traditional QCRA framework was implemented as a BN, constructed within a wastewater reuse scenario using published data, and refined through expert elicitation. The modular nature of BNs allow us to combine data from multiple sources with expert knowledge helping to compensate for the limited available empirical data, thus fulfilling QCRA requirements. The correctness of the model was verified through sensitivity analysis and by evaluating its applicability to real-world scenarios.

3.1. The chemical

Given its high frequency of occurrence (Crone et al., 2019; Kurwadkar et al., 2022; Kaboré et al., 2018), environmental persistence (Christensen et al., 2022), and established toxicity (Kudo and Kawashima, 2003; Anderson et al., 2019), PFOA was selected as the representative "worst-case" compound for this scenario.

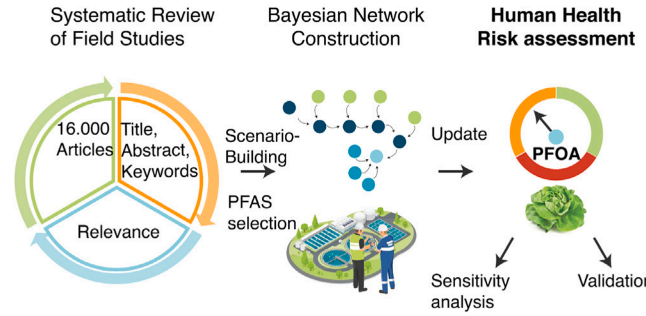

Fig. 1. Study outline.

3.2. The exposure scenario

This study considers a conservative exposure scenario in which wastewater containing PFOA is used to irrigate salad crops grown in soil, with wastewater delivered via sprinkler system every 2–4 days, following common agricultural practices. In this regard, only a limited number of studies have investigated the fate and uptake of such compounds in lettuce irrigated with wastewater. Therefore, our study builds upon the research by Blaine et al. (2014), which provides essential baseline data. The exposure route studied is ingestion through salad consumption. An additional scenario was also explored, considering farm workers during crop harvesting. In this case, the selected exposure route was unintended ingestion, due to limited data for other routes (i.e. inhalation or dermal contact). Since the link between PFOA exposure and human health effects remains uncertain, we based the reference dose on the international epidemiological range reported by Burgoon et al. (2023).

4. Materials and methods

4.1. Meta-analysis

Papers were selected using the following search string in SCOPUS database in 2024: PFAS and "wastewater treatment plant". The selected keywords were identified as they yielded scientific publications focused on more than one PFAS, while not excluding publications that worked with only one wastewater treatment plant, as in Ilieva et al. (2024). Papers were collected between 2006 and 2024, and limited to research papers written in English. The initial research yielded to 16.000 papers. To further refine the research, articles were selected based on title, abstract, and keywords. Subsequently, relevance criteria were applied, examining whether the studies reported data on treatment system efficiency, were based on real-world data or laboratory experiments, and focused on conventional wastewater treatment processes. Through successive iterations of this procedure, the research field was further narrowed down using keywords from the selected articles. Finally, approximately 40 articles were identified, that met the following inclusion criteria: (a) focused exclusively on wastewater treatment plants (excluding drinking water treatments and sludge), (b) included measurements for both influent and effluent or reported treatment step efficiency, (c) provided data for individual PFAS compounds, (d) be performed at full-scale and (e) present conventional treatment schemes. From each selected study, data were extracted on PFAS removal efficiencies across individual treatment steps, categorized as follows: primary (physical processes such as screening, grit removal, and sedimentation), secondary (biological treatments including activated sludge, SBRs, and MBRs), tertiary (advanced processes such as GAC/PAC adsorption, AOPs, ion exchange, and membrane filtration), and disinfection (e.g., chlorination, ozonation, UV). In addition to removal efficiencies, influent and effluent concentrations were collected for each individual PFAS, including detection

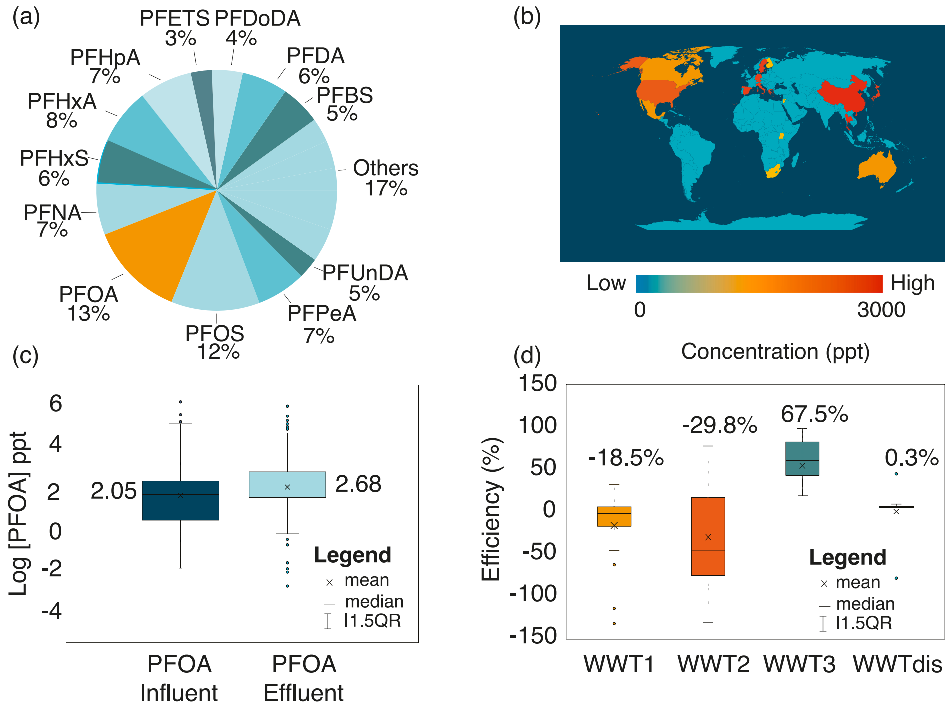

Fig. 2. Meta-analysis results. (a) Predominant PFAS identified in influent and effluent water matrices; (b) global distribution of PFOA in wastewater samples; (c) and (d) box plots illustrating PFOA concentrations in influent and effluent, respectively, along with the corresponding removal efficiencies of wastewater treatment processes. The treatment stages are denoted as WWT1 (primary treatment), WWT2 (secondary treatment), WWT3 (advanced treatment), and WWTdis (final disinfection).

limits. From the meta-analysis results, four PFAS were selected due to their prevalence in both influent and effluent waters, as illustrated in Fig. 2a. These include two short-chain PFAS — perfluorohexanoic acid (PFHxA) and perfluorohexanesulfonic acid (PFHxS)— and two long-chain PFAS -perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS). Among these, PFOA stands out for its ubiquitous detection across all examined regions, as shown in Fig. 2b. The distribution of influent and effluent PFOA concentrations is presented through box plots in Fig. 2c. As shown in Fig. 2c, the average concentration of PFOA (over n=457 counts) in effluent (54 ± 172 ppt) exceeds that in influent (43 ± 184 ppt), indicating poor removal efficiency in conventional WWTPs (Eriksson et al., 2017; Guerra et al., 2014), as further supported in Fig. 2d. This behavior underscores the role of WWTPs as both recipients and conduits of PFAS into aquatic environments (Kibambe et al., 2020; Xiao et al., 2024).

4.2. QCRA

As in Beaudequin et al. (2017), a deterministic QCRA model of risk of PFOA exposure was constructed using @XLSTATA by Lumivero (XLSTAT, 2021) with points estimates from literature. Following validation, a stochastic model was developed from the deterministic model, using distributions derived from the peer-reviewed studies or triangular distributions with maxima and minima collected from the literature when informative distributions where not available, using Python v.3.7.1. Beyond the choice of preferring informative priors that reflect a certain confidence or restriction on parameters, there is an implicit acknowledgment of the existence of a potential risk associated with the modeled scenario, as discussed in Seis et al. (2024). 10.000 values were randomly generated from each distribution using Markov Chain Monte Carlo (MCMC) sampling methods, via Python package PyMC v.5.5.0. Threshold values for parent node states were selected based on percentiles (literature-derived), equal-probability binning or on the base of Australian Guidelines (Huh, 2005; Beaudequin et al., 2016). In contrast, the conditional probabilities for child nodes were calculated using Bayes' rule by discretizing the data into states according to the selected threshold values. The BN was constructed using the Python tool pgmpy (Ankan and Textor, 2024).

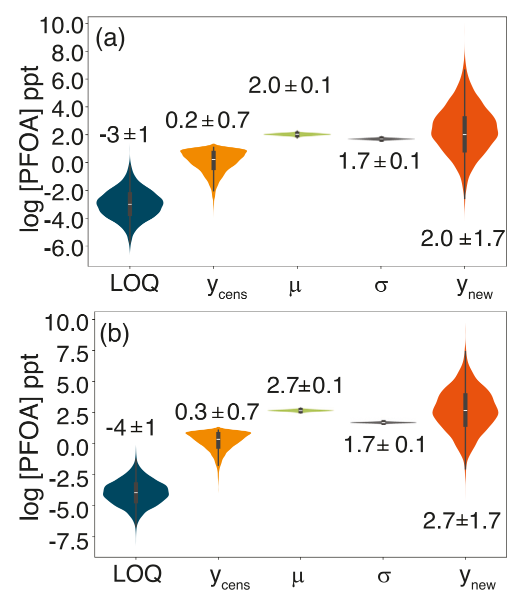

Fig. 3. Violin plots for posterior predictive distribution of parameters about PFOA concentration in a. influent and b. effluent.

4.2.1. Modeling PFOA concentration in treated wastewater

The exposure data collected from literature review indicated a percentage of 10% below the limit of quantification (LOQ), which is higher than the 5% threshold indicated by the EPA, above which substitution with LOQ/2 or 0 is not recommended (Sahoo et al., 2024). Such values,

Table 1
Likelihoods and priors distributions assumed for modeling censored input and output concentrations.

Parameters	Distribution	Hyperparameters	Description	References
μ	Uniform (a,b)	a=[C_{min}], b=[C_{max}]	Prior	[a]
std	Half Normal(σ)	$\sigma = 1$	Prior	[a]
LOQ	Normal (μ, σ)	$\mu = [C_{min}]$, σ=1	Prior	[a]
Y_{cens}	Uniform (a,b)	a=LOQ_{min}, b=LOQ_{max}	Prior	[a]
likelihood	Normal	$\mu = \mu$, $\sigma =$ std	Likelihood	[a]
likelihood$_{cens}$	Potential	log CDF using Y_{cens}	Likelihood	[a]
y_{new}	Normal	$\mu = \mu$, $\sigma =$ std	Posterior	[a]
y_{cens}	Truncated Normal (μ, σ, a,b)	$\mu = \mu$, $\sigma =$ std, a=LOQ_{min}, b= LOQ_{max}	Posterior	[a]

[a] Suzuki et al. (2020).

which fall below a quantifiable threshold and cannot be precisely measured, are referred to as left-censored data. The high percentage of censored data leads to uncertainty in estimating PFOA exposure; to avoid to add bias by replacing arbitrary values, a new approach was employed to estimate values under LOQ, using the Markov Chain Monte Carlo (MCMC) method, following a protocol similar to that proposed in previous studies (Suzuki et al., 2020; Mentzel et al., 2022b). To estimate the model parameters used in the parameterization of the BN, Bayesian inference was applied under defined assumptions. It was assumed that the (natural logarithm-transformed) concentration data, both influent and effluent, followed a normal distribution. The prior distribution for the mean was assumed to be uniform, whereas the standard deviation was assigned a half-normal prior. The hyperparameters of these prior distributions — mean (μ) and standard deviation (σ)— were derived from a meta-analysis. The left-censored data (Y_{cens}), which fall between the lowest and highest LOQ values, were estimated through inference using the Python library PyMC3 with the No-U-Turn Sampler (NUTS), configured with 2000 iterations, 1000 warm-up steps, 4 chains, and thinning set to 2. The cumulative distribution function (CDF) was employed to represent the likelihood for censored observations. Additionally, new random values (y_{new}) were generated for the posterior predictive check. The prior distributions and modeling assumptions are reported in Table 1. The results of the algorithm are consistent with those of the method proposed by Mentzel et al. (2022b), where classical Monte Carlo methods are employed. After the MCMC iteration finished, three parameters (μ, σ, and LOQ) employed for the inference calculations, had converged. In all calculation results, $\hat{R}$, which is the ratio of inter-chain variance to intra-chain variance, satisfied 1.1 or less, which is a general criterion of convergence. Moreover, the relative Monte Carlo deviation (MCSE) also satisfied general criteria (0.1 or less). The posterior mean estimates for input and output concentrations (Fig. 3) closely matched those calculated through a similar method (Suzuki et al., 2020), with a relative deviation of 6%, further supporting our approach. This suggests the possibility of employing this protocol in similar contexts, where uncertainty may affect a proper evaluation. The results of the algorithm were used for both deterministic and stochastic dataset construction. Specifically, PFOA concentration throughout the wastewater treatment chain was modeled starting from the input concentration as (Specker et al., 2025):

$$C_n = C_{n-1} \cdot (1 - T_n(\%)) \tag{3}$$

where C_n and C_{n-1} are the concentrations after and before treatment n, respectively, while $T_n(\%)$ indicates the treatment efficiency.

4.2.2. Modeling of risk

The risk associated with PFOA exposure through the ingestion of salad irrigated with reclaimed water was modeled as follows. Specifically, the Estimated Daily Intake (EDI) was calculated using the expression:

$$EDI = \frac{C_{\text{effluent}}(ng/L) \cdot BAF(ng/ng_w) \cdot DC(g/(g \cdot day)) \cdot V_w(L)}{weight(kg)} \tag{4}$$

where C_{effluent} is the effluent concentration, BAF is the bioaccumulation factor estimated from the paper of Blaine et al. (2014) for lettuce grown in soils with different organic contents (0.4% to 6%) and consumed after washing, DC is the daily consumption of salad per plant (NRMMC-EPHC-AHMC, 2006). V_w is the watering volume required for lettuce plant growth, ranging from 4 to 45 L depending on the season (Blaine et al., 2014), while body weight is assumed to be 70 kg, as common practices (Bleam, 2012). The final hazard quotient (HQ) was estimated according to Eq. (1), using RfD values ranging from 10 ng/L to 70 ng/L, as estimated in the study by Burgoon et al. (2023).

4.3. Bayesian network

The structure of the BN was derived from the QCRA process. Nodes selection was conducted using a hybrid approach that combined expert knowledge with data-driven scoring methods. The design of the network was informed by the multi-barrier approach, encompassing the entire water reuse process. This included four nodes representing treatment stages: WWT1 (primary treatment), WWT2 (secondary treatment), WWT3 (polishing treatment), and WWTdis (final disinfection), as well as one node representing a post-treatment health protection measure, included in V_w. Prior probability distributions were sourced from published literature (Simonetti et al. 2025a, for other references see Table 3). As previously stated, threshold values for parent node states were either derived from meta-analytical data or determined using equal-probability binning, as summarized in Table 3. Conditional probability tables (CPTs) for child nodes were computed using Bayes' rule, following the discretization of continuous variables into three states: low, medium, and high, based on the selected thresholds. All nodes were discretized into three states, with the exception of the final node (HQ), which was discretized into five states to enable a more granular representation of the hazard quotient. The BN was implemented using the pgmpy Python package (Ankan and Textor, 2024). An example of conditional probability table for PFOA concentration (C1) before the primary treatment (WWT1) is provided in Table 2. From Table 2 it can be seen that the probability of C1 being "High" when C_{influent} is "High" and WWT1 is "Low" is 0.996. Likewise, the probability of C1 being "Low" when both C_{influent} and WWT1 are "Low" can be seen to be 0.750. It can also be seen, reasonably, that it would be impossible (P=0) to achieve a very low C1 when C_{influent} is "High" and WWT1 is "Low". The network shown in Fig. 4 represents the prior or baseline state of knowledge, which can be updated as new water quality data become available. At this baseline level, the probability assigned to each node state reflects the estimated likelihood of that state occurring. To study the effect of new evidence introduced in the BN, the percentage change of each response node was computed as (Beaudequin et al., 2017):

$$\frac{P_{baseline} - P_{evidence}}{P_{baseline}} \% \tag{5}$$

where P_{baseline} is the probability of occurrence of response node states under baseline network conditions before new evidence is introduced and P_{evidence} is the probability of a state occurring after new evidence is introduced in the network.

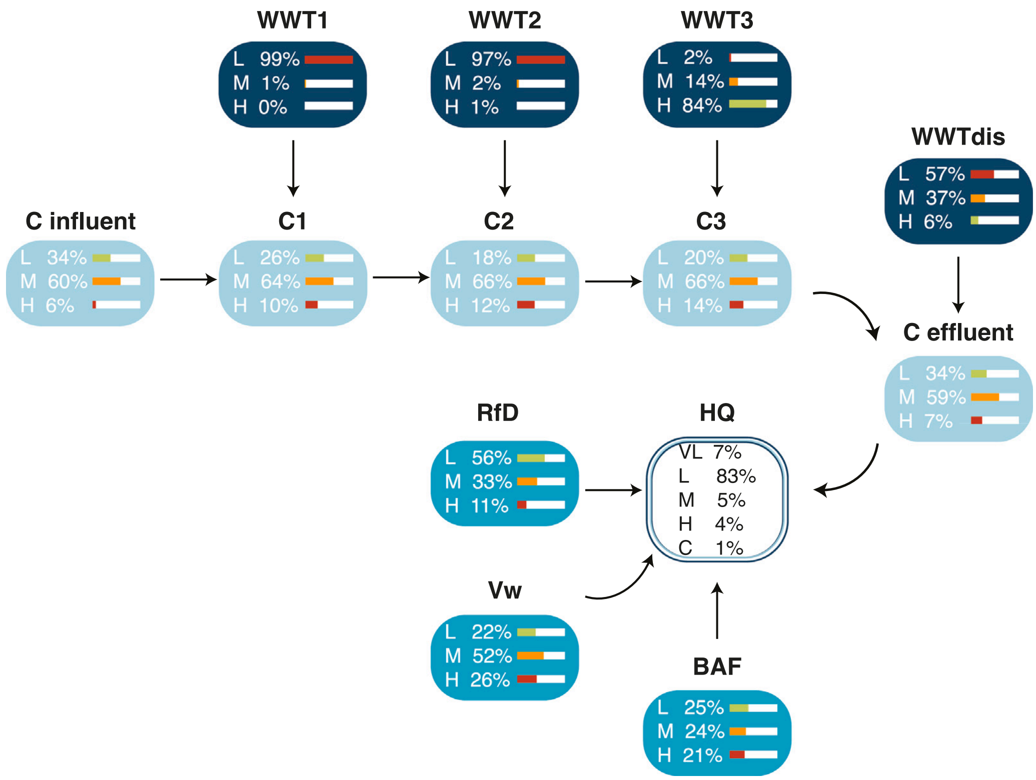

Fig. 4. A baseline Bayesian network was constructed to represent the risk of PFOA exposure through salad consumption. This network can be dynamically updated as new water quality data become available. At the baseline stage, the probabilities assigned to each node state represent the estimated likelihood of those conditions occurring.

Table 2
Conditional Probability Table (CPT) for the effluent concentration after the first treatment stage (C1), based on the influent concentration and the removal efficiency of the primary treatment.

$C_{influent}$		Low			Medium			High		
WWT1		Low	Medium	High	Low	Medium	High	Low	Medium	High
C1	Low	0.750	1	0	0.001	0.083	0	0	0	0
C1	Medium	0.250	0	0	0.940	0.917	0	0.004	0.250	0
C1	High	0	0	0	0.058	0	0	0.996	0.750	0

4.3.1. Validation of the Bayesian network

During the structural development and evaluation phase, the deterministic QCRA model was formulated and reviewed in collaboration with representatives from the water utility sector, public health authorities, and academic researchers. A preliminary validation of the model outputs was conducted by comparing them against published benchmark values from the literature. Based on this conceptual framework, a BN structure was constructed. Prior elicitation, node discretization, and parameterization were informed by a combination of meta-analytic results, expert opinion, and peer-reviewed estimates. The BN was initially assessed using an in-sample posterior predictive check, referencing literature-based data points for internal consistency, as shown in Fig. 5. Subsequently, external validation was performed under real-world exposure conditions by applying the trained BN model to an independent dataset derived from field measurements.

4.4. Field - monitoring

Data were collected at the influent and effluent of two Italian WWTPs (> 50,000 PE), operating with conventional treatment schemes and designated for future water reuse purposes. Over the course of one year, a monitoring program targeting per- and polyfluoroalkyl substances (PFAS), including PFOA, was conducted through monthly sampling, using an UHPLC-MS/MS protocol similar to that of Mancini et al. (2023).

4.5. Standards

Optima LC-MS grade acetonitrile, ultrapurewater, and methanol were purchased from Biosolve (Valkenswaard,Netherlands). LC-MS grade (> 99%) ammonium acetate (CH_2O_2) was purchased from VWR International Srl (Pennsylvania, USA). Vials (Phenomenex, part.no.AR0-3611-12) were purchased from Phenomenex (Torrance, USA). Analytical standards including the PFAC-24PAR technical solution and the MPFAC-24ES mass-labeled technical solution (1,2 mL, 50 μg/mL in methanol), were purchased from Wellington Laboratories (Guelph, ON, Canada), kept away from PFAS packaging and material during storage. Calibration solutions, with concentrations of 1–1000 ng/L, were prepared by serial dilutions of the stock solution in 30:70 (v/v) methanol/ ultra pure water.

4.6. Instrumental analysis

Analysis was carried out using a Thermo Scientific UHPLC UltiMate 3000 system coupled with a Thermo Scientific TSQ Altis triple quadrupole mass spectrometer and equipped with an ESI ionization probe. Chromatographic separation was performed on a Luna Omega PS C18 analytical column (Phenomenex, P/N 00D-4752-AN; 100 × 2.1 mm, 1.6 μm particle size), protected by a Luna C18 guard column (Phenomenex, P/N 00A-4252-Y0; 5 μm, 100 Å, 30 × 3 mm). Mass

Table 3
Variables distributions, states and ranges. Priors distributions were defined for parent node in underlying model: normal (mean, standard deviation); triangular (minimum, most likely, maximum); uniform (minimum, median, maximum). Threshold values were derived using percentile-based discretization (PBD) applied to literature-reported data, or were based on equal-probability binning when no reference values were available.

Variable	Unit	Distribution	Thresholds	discretization	References
C_{influent}	ng/L	LogNormal (2.05, 1.66) truncated at 0	[4 100]	PB (literature-derived)	[a]
WWT1	%	Triangular (−132,−54,30)	[20 40]	PB (literature-derived)	[b]
WWT2	%	Triangular (−131,−66,99)	[20 40]	PB (literature-derived)	[c]
WWT3	%	Triangular (−131,−66,99)	[20 40]	PB (literature-derived)	[d]
WWTdis	%	Triangular (−131,−66,99)	[20 40]	PB (literature-derived)	[e]
Vw	L	Uniform (4, 45)	[17 30]	equal probabilities	[f]
Ving	mL/event	Triangular (0.5,1,2)	[0.7 1.5]	equal probabilities	[g]
N	event/h	Triangular (0,4,26)	[3 10]	equal probabilities	[h]
TE	–	Uniform (0.1 1)	[0.3 0.7]	equal probabilities	[i]
BAF	ng/ng_w	Uniform (0.2, 0.6)	[0.3 0.5]	equal probabilities	[j]
RfD	ng/day-kg	Triangular (10, 10, 70)	[30 50]	equal probabilities	[k]
C1	ng/L	–	[4 100]	PB (literature-derived)	[l]
C2	ng/L	–	[4 100]	PB (literature-derived)	[m]
C3	ng/L	–	[4 100]	PB (literature-derived)	[n]
C_{effluent}	ng/L	–	[4 100]	PB (literature-derived)	[o]
HQ	–	–	[0.0005 0.11 0.22 1]	PB (literature-derived)	[p]

[a] Thompson et al. (2022), Gewurtz et al. (2024), Moneta et al. (2023), Schaefer et al. (2023), Szabo et al. (2023), Miserli et al. (2023), Coggan et al. (2019), Wang et al. (2020), Bossi et al. (2008).
[b] Forsberg (2022), Arvaniti and Stasinakis (2015), Schultz et al. (2006), Sinclair and Kannan (2006), Yu et al. (2009), Gewurtz et al. (2024), Zhang et al. (2013).
[c] Forsberg (2022), Arvaniti and Stasinakis (2015), Yu et al. (2009), Schultz et al. (2006), Gewurtz et al. (2024).
[d] Forsberg (2022), Arvaniti and Stasinakis (2015), Gewurtz et al. (2024), Zoumpouli et al. (2023), Veciana et al. (2022), Thompson et al. (2011), Choe et al. (2022).
[e] Forsberg (2022), Arvaniti and Stasinakis (2015), Appleman et al. (2014), Gewurtz et al. (2024), Dai et al. (2019), Thomas et al. (2020).
[f] Bleam (2012).
[g] Fuhrimann et al. (2016), Organization (2006).
[h] Ng et al. (2016).
[i] Rohrer et al. (2003).
[j] Bleam (2012).
[k] Bleam (2012).
[l] Thompson et al. (2022), Gewurtz et al. (2024), Schaefer et al. (2023), Szabo et al. (2023), Lenka et al. (2022), Miserli et al. (2023), Wang et al. (2020), Bossi et al. (2008).
[m] Thompson et al. (2022), Gewurtz et al. (2024), Schaefer et al. (2023), Szabo et al. (2023), Lenka et al. (2022), Miserli et al. (2023), Wang et al. (2020), Bossi et al. (2008).
[n] Thompson et al. (2022), Gewurtz et al. (2024), Schaefer et al. (2023), Szabo et al. (2023), Lenka et al. (2022), Miserli et al. (2023), Wang et al. (2020), Bossi et al. (2008).
[o] Thompson et al. (2022), Gewurtz et al. (2024), Schaefer et al. (2023), Szabo et al. (2023), Lenka et al. (2022), Miserli et al. (2023), Wang et al. (2020), Bossi et al. (2008).
[p] Mentzel et al. (2022b).

spectra were recorded in negative ion mode. The total run time was 22 min, with a flow rate of 0.3 mL/min and a gradient elution composed of two mobile phases: water with 5 mM ammonium acetate (A) and acetonitrile (B), following this program: 98% eluent A for 0.5 min; from 0.5 to 14 min eluent A was decreased to 5% and held costant for 2 min; after that, eluent A was raised to 98% in 0.1 min and held at 98% until the end of the run. The column temperature was 40 °C, the internal autosampler temperature was set at 25 °C and the injection volume was 100 μL. The mass spectrometer parameters in negative ionization mode were as follows: spray voltage −2.5 kV, sheath gas flow rate 50 a.u., auxiliary gas flow rate 10 a.u., sweep gas flow rate 1 a.u.; the ion transfer tube was set at 325 °C and the vaporizer at 300 °C. MS/MS analysis was performed in multiple reaction monitoring (MRM) mode. The monitored mass transitions are 413–369 (Collision Energy, CE, of 9 V) and 413–219 (CE of 15 V), respectively. Wastewater samples were diluted with methanol (70:30, v/v) and spiked with formic acid (0.1%), after analysis. Reproducibility and precision were assessed by including blank and quality control (QC) samples in each analytical run. The method's limit of quantification (LOQ) was determined to be 2.5 ng/L.

5. Results

5.1. Sensitivity analysis

To evaluate the structural validity and robustness of the BN, a sensitivity analysis was conducted. This procedure involved systematic perturbation of the marginal distributions of the input nodes to quantify their influence on the posterior distribution of the target variable, namely the hazard quotient (HQ). Specifically, we varied the probability that each of our input variables, C_{influent}, WWT1, WWT2, WWT3, and WWTdis, was in the "High" state, then recorded the resulting change in the probability that HQ is in the "High" state. The results of this analysis are shown in Fig. 6. As expected, increasing the probability of a high influent concentration raises the likelihood of a high HQ state, whereas improving treatment effectiveness at any stage reduces that likelihood. This indicates that upstream contaminant load is the dominant driver of risk in the model. Conversely, improvements in treatment performance are associated with a reduction in the probability of high-risk outcomes. Moreover, Fig. 6 shows that the offset associated with the scenario where the advanced treatment (WWT3) is completely ineffective results in the highest baseline risk level compared to all other treatment stages. This suggests that, in contamination scenarios, the absence or failure of tertiary/quaternary treatments substantially amplifies the overall risk, highlighting their critical role in system resilience.

5.2. Scenarios assessment

In addition to their descriptive capacity to represent complex risk pathways under conditions of uncertainty, BNs offer a particularly valuable feature: the ability to simulate a range of scenarios by varying exposure levels and risk mitigation parameters. In the following sections, we explore five distinct scenarios. Scenario I simulates a PFOA contamination event. Scenario II examines a modification of the treatment chain. Scenario III evaluates the potential impacts of climate change, with a specific focus on a prolonged drought period. Scenario IV assesses the risk of unintended ingestion during crop harvesting, while Scenario V highlights the importance of using personal protective equipment (PPE).

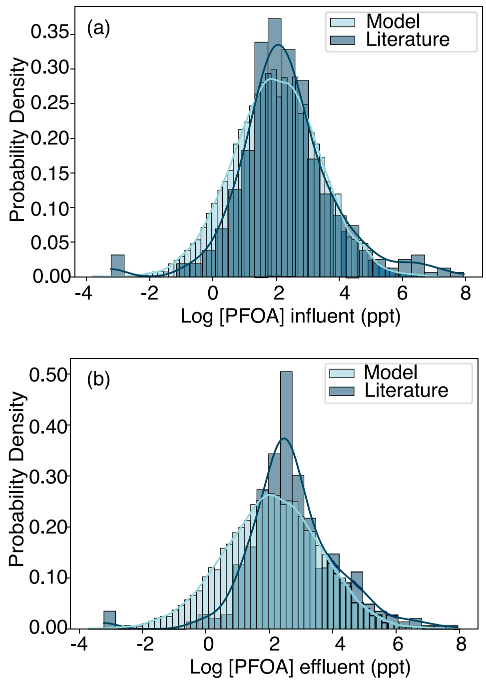

Fig. 5. Histograms of generated samples of PFOA concentrations in influent and effluent, assumed to follow a log-normal distribution with estimated parameters. The posterior predictive distributions were compared with observed data from the literature as part of a posterior predictive check.

5.2.1. Scenario I: PFOA contamination without risk mitigation

In this scenario, it was considered a study area experiencing high concentrations of PFOA, due a persistent spill-over of this substance from a former chemical factory (Giglioli et al., 2023). In this case, PFOA concentration can reach very high values, ranging between 0.2 ppb up to 7.5 ppb in influent water, as reported in many literature case studies (Moneta et al., 2023; Gagliano et al., 2020; Vo et al., 2020). This evidence was added to the network, by setting the PFOA influent concentration node to 100% “High”, as observable in Fig. 7a. In accordance with the results observed in the sensitivity analysis, the probability of a high risk of exposure to PFOA increases substantially, reaching 34% “High” and 59% “Critical”. A high influent concentration of PFOA in the WWTP can pose a significant health risk due to the consumption of salad irrigated with treated effluent. This finding indicates that current treatment schemes are insufficient to effectively mitigate PFOA contamination events. At the same time, it highlights the urgent need for innovative technologies and integrated management strategies to effectively address PFAS pollution.

5.2.2. Scenario II: Treatment change

PFOA is recognized for its persistence and occurrence in wastewater, with poor removal during primary and secondary treatment processes (Moneta et al., 2023; Thompson et al., 2011). Many water utilities lack tertiary/quaternary treatment systems due to high operational and maintenance costs. In this context, a conventional treatment scenario where advanced treatment is not in operation is considered. This evidence was added to the network, by setting the removal efficiency node WWT3 to 100% “Low”, as observable in Fig. 7b. Results indicate a slight increase in the probability of observing a “High” and “Critical” HQ, rising to 9% and 2%, respectively. This suggests that, under moderate influent concentrations of PFAS, the absence or failure of polishing treatments does not necessarily lead to exceedance of risk thresholds. However, considering both the previous pollution scenario and the results of the sensitivity analysis, it becomes evident that tertiary/quaternary treatments play a crucial role as a mitigation barrier in the event of a contamination incident. Their implementation, therefore, remains a key element in reducing health risks associated with PFAS exposure via reclaimed water.

5.2.3. Scenario III: Drought

Climate change is intensifying droughts globally, increasing the need for irrigation to support agriculture. In this scenario, we hypothesized an extended dry period during the summer, similar to that of 2024. This condition was incorporated into the network by setting the watering volume (V_w) to 100% “High”, as displayed in Fig. 8. Under these conditions, the probability of observing a “High” Hazard Quotient increases by 125% following the addition of new evidence, while the probability remain low at 9%. This outcome suggests that increased water volumes do not significantly elevate the risk under standard operating conditions. However, this assumption represents a simplification. In reality, cumulative exposure and plant uptake could be influenced by prolonged or intensified irrigation, particularly under drought conditions. Further experimental data are needed to assess whether irrigation practices or water stress can significantly alter BAF values in edible crops.

5.2.4. Scenario IV: Unintended ingestion during crops harvesting and handling

To further evaluate the capability of the BN to represent additional exposure scenarios, we modeled an extra exposure route related to wastewater reuse in agriculture. The JRC technical guidelines on “Water Reuse Risk Management for Agricultural Irrigation Schemes in Europe” (Maffettone et al., 2022) identify dermal contact, unintended ingestion of soil and water, and inhalation as possible exposure routes during the harvesting of crops irrigated with spray nozzles. Overall, the unintended ingestion of contaminated water through the hand-to-mouth ingestion pathway was selected, while the following exposure pathways were excluded: (i) ingestion of contaminated soil, (ii) dermal contact, and (iii) inhalation, due to the lack of empirical data to define a plausible scenario. The BN structure was adapted to assess the potential health risk associated with this exposure pathway, leaving the entire treatment chain unchanged and modifying only the final part. For this scenario, the target population consists of 70-kg workers who work 8-hours per day in the field. The Estimated Daily Intake (EDI) for this scenario was calculated as:

$$EDI = \frac{C_{\text{effluent}}(ng/L) \cdot t_{work}(h/day) \cdot V_{ing}(10^{-3}L/event) \cdot TE \cdot N(event/h)}{weight(kg)} \tag{6}$$

where t_{work} is the exposure time, assumed to be 8 h; TE represents the PFOA transfer efficiency from water to hands; and N is the number of hand-to-mouth contacts per hour. TE was assumed to be uniformly distributed between 0.1 and 1, while N was modeled using a triangular distribution with bounds derived from the study by Ng et al. (2016). The ingestion volume (Ving) for hand-to-mouth transfer was estimated using a triangular distribution, following the approach described in literature (Organization, 2006; Busgang et al., 2018). The HQ was calculated according to Eq. (1). The modified BN is displayed in Fig. 9a.

The baseline results show that the “Critical” category has the highest individual probability (50%), suggesting that the investigated route of exposure may represent a relevant concern. Compared to the crop consumption pathway (Fig. 4), the probability of Medium-Critical HQ levels increases by approximately a factor of 9. To assess the relative contribution of the two exposure routes, a severity index S was computed as (Eq. (7)):

$$S = \sum s_i p_i \tag{7}$$

where s_i represents the ordinal severity score (1 = “Very Low” (VL); 5 = “Critical” (C)) and p_i the corresponding class probability. The

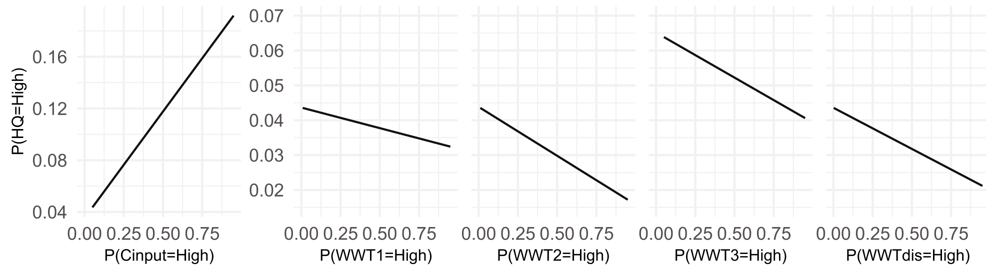

Fig. 6. Results of sensitivity analysis on the risk model for the four treatment nodes.

resulting severity indices were 4.2 for unintended ingestion and 2.1 for crop consumption, indicating that unintended ingestion should be considered the higher-priority pathway for risk assessment and potential mitigation planning. It should be noted that the reported relative contribution refers only to the two exposure routes modeled in this study, as other potentially relevant pathways could not be incorporated due to data limitations. Nevertheless, the proposed Bayesian QCRA framework shows potential for supporting broader total-risk assessments, which are of clear public interest.

5.2.5. Scenario V: Good behavioral practices in crop harvesting

In this scenario, the effect of using personal protective equipment (PPE) to safeguard farm workers safety was investigated. The node N, whose behavioral pathway is directly influenced by PPE use and proper handwashing practices, was set to 100% "Low", assuming an ideal full-compliance scenario where workers are equipped with appropriate PPE, including facial and hand protection (Fig. 9b). After updating the BN with this new evidence, the probability of HQ being in the "Critical" state decreases to 3%, while the probability of being in the "Low" state increases from 11% to 74%. These results highlight the relevance of preventive measures and good occupational practices in agriculture, significantly mitigating the risk.

5.3. Application in a real-world scenario

The proposed BN was applied to a real-world case study involving two municipal WWTPs located in central Italy. Influent and effluent concentration data, collected monthly over the course of a one-year monitoring campaign, were incorporated into the BN model. Notably, over 30% of the data, as shown in Fig. 10a-b, were below the method's limit of quantification (LOQ). Additionally, treatment efficiency data were unavailable due to the high associated costs, which introduced further uncertainty into the risk estimation process. Despite these limitations, the HQ values, calculated according to Eq. (1) and illustrated through the gauge plots in Fig. 10a-b, indicated an acceptable risk level for both WWTPs, with 84% and 81% of outcomes falling within the "Low" risk category, respectively, aligning with the low contaminant concentrations observed during the monitoring period. This demonstrates that the BN approach enabled a robust risk assessment even under conditions of limited and uncertain data, where the traditional QCRA approach was unusable.

6. Discussion

6.1. Main findings

A key finding of this study is that current treatment chains are not sufficiently effective in removing PFOA during contamination events. This result aligns with evolving regulatory frameworks, which increasingly emphasize the need for advanced treatment solutions in wastewater management, particularly for persistent and bioaccumulative substances. In particular, the European Directive 3019/2024, recently transposed by Member States, mandates the implementation of quaternary treatment for the removal of micropollutants. This requirement applies to large-scale treatment plants and those discharging into sensitive areas, as determined by a risk-based assessment in line with the precautionary principle. In this context, the model developed in this study highlights the critical role of advanced treatment technologies. Both tertiary and quaternary treatments are shown to be essential in mitigating risks associated with contamination events involving persistent pollutants such as PFOA and other PFAS. These findings further support ongoing research and policy development in the field of emerging contaminants.

6.2. Strengths and limitations: potential design variation

Over the past decade, there has been a growing interest in the application of BNs, driven by the recognition that both stakeholder involvement and uncertainty are critical components in integrated natural resource management (Castelletti and Soncini-Sessa, 2007). In the water sector, BNs have emerged as powerful tools, particularly due to their ability to integrate diverse information sources and capture system dynamics, thereby enhancing the understanding of complex environmental systems. This study has demonstrated that BNs can incorporate quantified uncertainties and variabilities in a more coherent, transparent, and flexible manner compared to traditional risk characterization approaches. In developing our methodology, we adhered to key recommendations for probabilistic risk estimation as outlined in the EMEA guidelines (Huschek et al., 2004). Our approach combines conventional deterministic assessment — based on the evaluation of the hazard quotient — with a more advanced QCRA, enabling the BN framework to represent uncertainties associated with PFAS quantification and their spatio-temporal variability (Wolf and Tollefsen, 2021). An additional advantage with respect to QCRA is that poor quality experimental data has little impact on a distribution function for PFAS concentration that is established from high quality prior information, and accurate quantification can be made also with small samples size, as in the case of PFOA. To facilitate end-user comprehension (e.g., regulators and stakeholders), the proposed BN approach presents outputs using intuitive visualizations, such as gauge plots, instead of cumulative probability distributions. This aligns with findings from Mentzel et al. (2022b), which emphasize that stakeholders are more inclined to engage with decision-support tools that rely on simple, familiar concepts and formats. A notable strength of our BN framework — to the best of our knowledge, the first of its kind in the context of PFAS-related risk assessment — lies in its potential for extensibility. Specifically, modeling two exposure scenarios demonstrated the operational scalability of the framework and its readiness for extension to additional exposure pathways, population groups, and reuse contexts, subject to data availability. Future applications may expand the network to simulate various water reuse scenarios by incorporating additional nodes, such as irrigation infrastructure and pre-use water storage. With further development, the model can also support risk evaluation across different reuse applications (e.g., urban green space irrigation), addressing diverse target populations — such as occupationally exposed

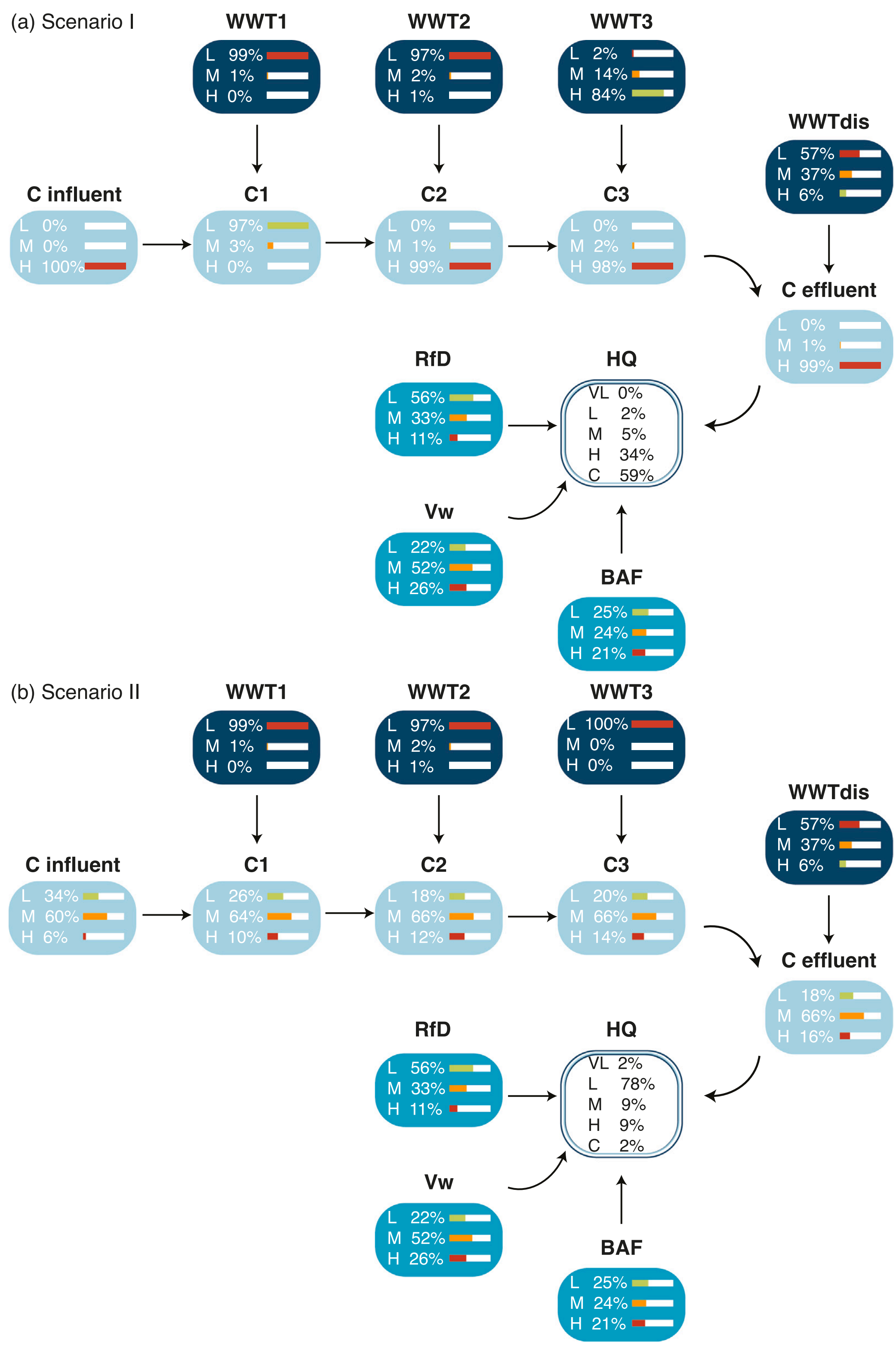

Fig. 7. Hazard quotients (HQs) after (a) PFOA contamination (Scenario I) and (b) after treatment change (Scenario II).

workers or children playing in treated areas — and multiple exposure pathways, both direct and indirect. Future enhancements may include the integration of detailed information regarding infrastructure characteristics, operational practices, and environmental conditions, thereby refining the case study representation. Additionally, the model could incorporate climate change impacts, which are increasingly relevant in long-term water resource planning. For example, precipitation data can be incorporated into the network either indirectly by estimating the volume of water used for irrigation which typically increases during dry periods and decreases with higher rainfall, as in this study, or directly, by modeling its impact on the inflow dynamics of sewage treatment systems. This approach allows the model to capture effects such as increased pathogen loads entering sewage treatment plants during heavy rainfall events, as demonstrated by Beaudequin et al.

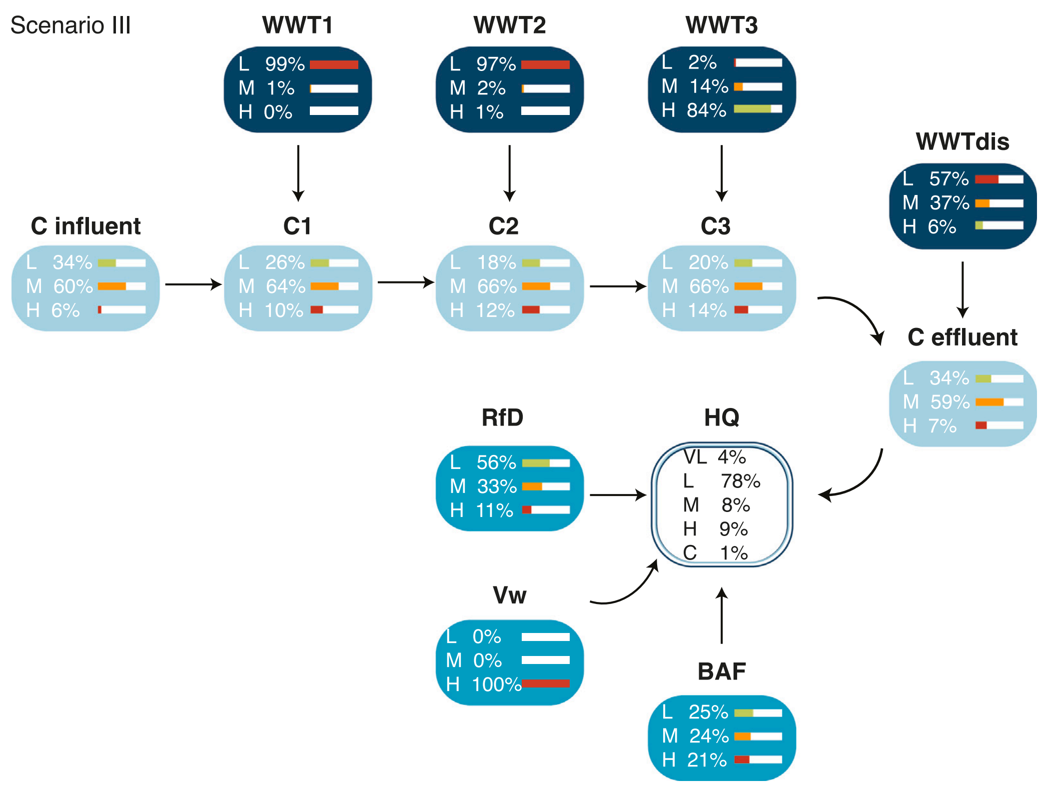

Fig. 8. Estimated hazard quotient (HQ) under drought scenarios involving increased water usage (Scenario III).

(2016). With respect to PFAS contamination, this study focused on the most prevalent and generalizable scenario, reflecting the current limitations and inconsistencies in available scientific data. At present, no regulatory thresholds have been established for PFAS concentrations in water intended for agricultural reuse or landscaping, further underscoring the need for precautionary and adaptive risk assessment tools (Simonetti et al., 2025a). As a final consideration, a key limitation of our approach is that the QCRA process is inherently chemical-specific and does not account for the potential synergistic or antagonistic effects — the so-called "cocktail effect" — of co-occurring PFAS and other contaminants. This limitation could be addressed in future work by incorporating hierarchical clustering techniques and leveraging more comprehensive toxicological data as it becomes available. Moreover, the framework could be extended to incorporate other contaminant classes, such as macropollutants and emerging contaminants, and further refined through expert elicitation processes. It should be noticed that several microbiological contaminants have already been evaluated using this approach (Donald et al., 2009; Beaudequin et al., 2016). This would enable the development of a multidisciplinary, integrated risk assessment approach, which is essential for supporting robust environmental and public health decision-making.

7. Conclusion

In this study, we proposed the integration of the Quantitative Chemical Risk Assessment (QCRA) tool into a Bayesian Network (BN) to describe the risk assessment process related to PFOA exposure along the wastewater reclamation chain. In this regard, a BN model representing the entire treatment chain was developed, and its applicability was tested through sensitivity analysis and simulation of common scenarios. In addition, we described and validated a novel approach for summarizing and analyzing left-censored PFOA concentration data in both influent and effluent of wastewater treatment plants (WWTPs). The proposed QCRA-BN model was applied to two wastewater Italian treatment plants, demonstrating consistent and reliable results. In conclusion, our study presents a potential framework for managing risk associated with PFAS exposure. The approach aims to address existing data gaps and support decision-makers through a structured and practical process — from water reuse considerations to the integration of treated effluent into the broader value chain.

CRediT authorship contribution statement

Federica Simonetti: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Methodology, Investigation, Data curation, Conceptualization. **Nicoló Ciuccoli:** Validation, Software, Methodology. **Ankur Ankan:** Validation, Software, Methodology. **Marco Mancini:** Validation, Methodology, Investigation. **Mario Castellani:** Validation, Methodology, Investigation. **Massimiliano Sgroi:** Validation, Supervision. **Francesco Fatone:** Validation, Supervision. **Valentina Migliorati:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Investigation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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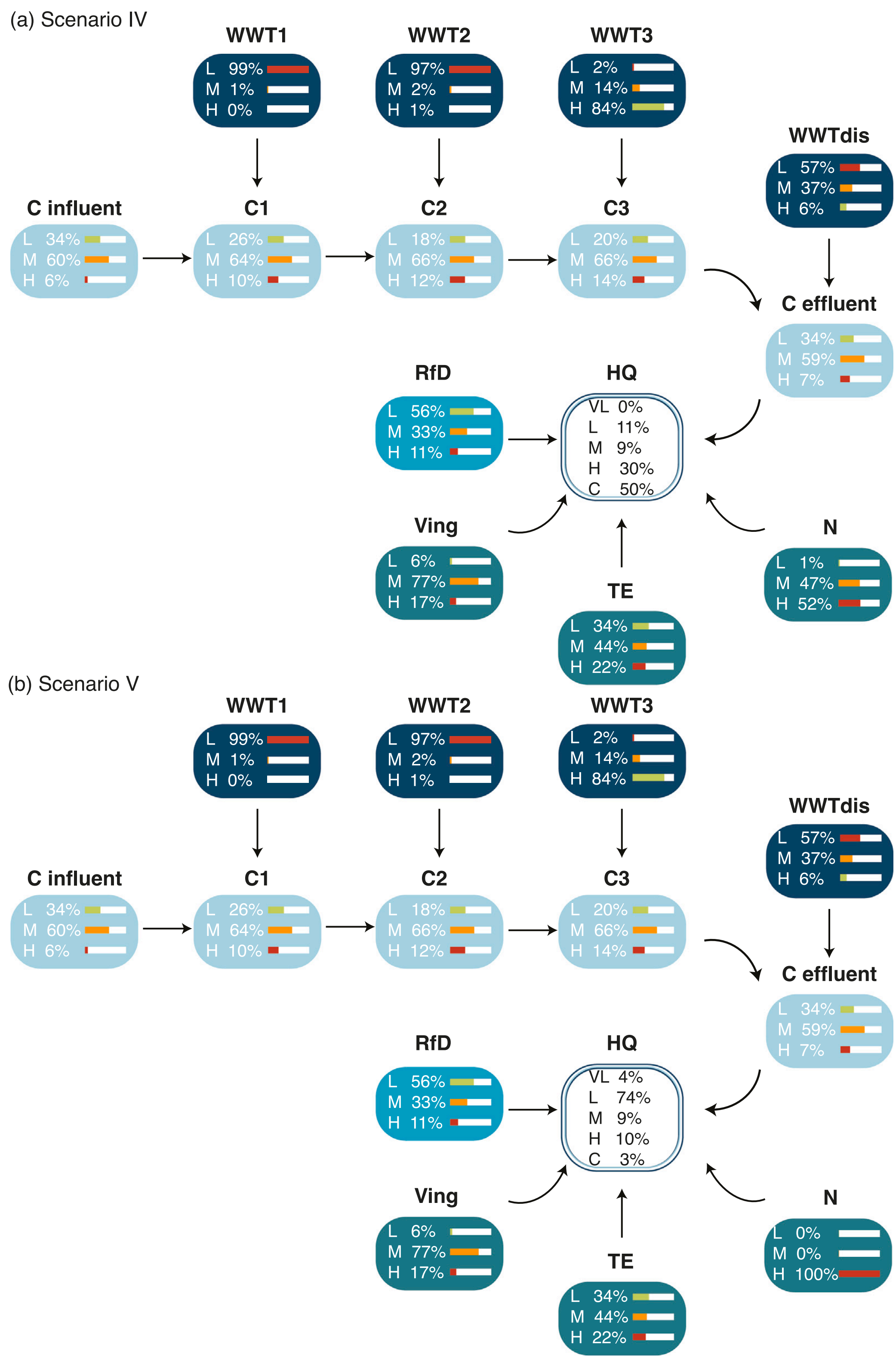

Fig. 9. Estimated hazard quotient (HQ) under (a) unintended ingestion of water by agricultural workers during crop harvesting (Scenario IV), (b) reduced exposure due to the use of personal protective equipment (PPE) (Scenario V).

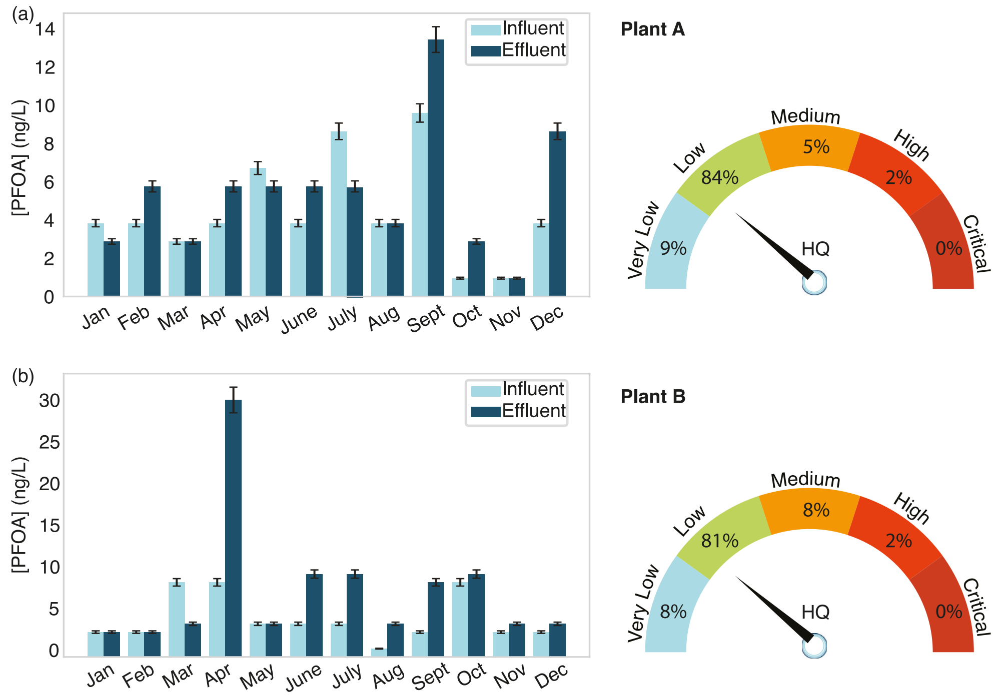

Fig. 10. Influent and effluent concentrations measured at plants A and B, with corresponding gauge plots showing the estimated Hazard Quotients (HQs).

Data availability

Data will be made available on request.

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