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Original Article

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Spatially referenced environmental exposure model for down-the-drain substance emissions across European rivers for aquatic safety assessments

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Abstract

A spatially referenced environmental exposure model for down-the-drain substance emissions was developed for Europe, including the 27 European Union Member States, Norway, Switzerland, and the United Kingdom. The model builds upon the global modeling framework that leverages the well-established iSTREEM model for the United States and further expands global coverage of the framework. The data are parameterized using European Union data on wastewater treatment plants, locations, infrastructure, and global spatial datasets on population and river flow rates and routing. The model provides substance concentration distributions based on the spatial variability of these parameters across Europe while taking into account river connectivity, chemical routing between rivers, and in-stream decay. Chemical-specific model inputs include wastewater treatment removals, in-stream decay rates, and emissions. The model is demonstrated for four case study chemicals that are used in consumer products with down-the-drain disposal routes: linear alkylbenzene sulfonate and alkyl sulfate are common surfactants used in laundry detergents, and oxybenzone and octinoxate are ultraviolet (UV)-filters used in personal care products. Monitoring data were collected to represent spatial variability across Europe as a comparison to modeled values. Modeled concentrations were found to be predictive while still being conservative, with 90th percentile modeled concentrations agreeing with monitored concentrations within a factor of two to eight across the case study substances. We further demonstrate how the model can be applied in prospective safety assessments by comparing modeled concentrations to previously established predicted no-effect concentrations, and also demonstrate how the model is consistent with tiered risk assessment approaches when compared to the monitoring data assessments.

Keywords: aquatic exposure model, down-the-drain, spatial variability, environmental safety assessment, Europe

Introduction

Spatially resolved aquatic exposure models have emerged to address the complexities of estimating aquatic exposure concentrations for consumer product chemicals disposed of down-the-drain. They are critical tools for assessing risks and enabling spatially explicit predictions of chemical emissions and in-stream concentrations. The iSTREEM model, originally developed for the United States (Kapo et al., 2016), leverages a robust, publicly available framework that estimates chemical concentrations in wastewater treatment plant (WWTP) effluents and receiving streams using high-resolution river flow data. By incorporating critical fate processes, such as in-stream chemical decay and downstream routing of chemical concentrations, iSTREEM provides additional realism and a comprehensive approach to aquatic exposure modeling. The United States version of the model was later expanded to parts of Canada (Ferrer and DeLeo, 2017) and has been leveraged in environmental safety assessments across several applications such as ingredients in cleaning and personal care products (Burns et al., 2021, 2022; Cowan-Ellsberry et al., 2014; Dawson et al., 2022; Fuchsman et al., 2022). The iSTREEM web platform was further expanded into a framework for global expansion to extend the geographic scope and be adaptable to diverse regions with varying population densities, wastewater treatment infrastructures, and geographic characteristics (McDonough et al., 2022). The global model framework was demonstrated for China and Japan, positioning the iSTREEM global framework as a key tool for addressing the complexities of down-the-drain chemical exposures in a consistent manner across global geographies and populations (McDonough et al., 2022). This paper builds upon these previous advancements by extending the global framework to Europe, encompassing continental-level exposure assessments across the European Union (EU) Member States, Norway, Switzerland, and the United

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Kingdom. While spatially resolved models have been developed for specific European countries (e.g., Kehrein et al., 2015; Kilgallon et al., 2017), the model presented in this article extends the area to cover 30 countries (or states) in Europe while also accounting for river connectivity across the continent allowing for transboundary river flow and transport processes.

Key inputs for down-the-drain aquatic exposure modeling are population, per capita water use or wastewater generation, wastewater treatment removal, and river flow which are combined with chemical emissions to arrive at a predicted environmental concentration (PEC) (Vamshi et al., 2025). Typical "unit-world" models represent these inputs for a region as single values and provide deterministic exposure estimates or PECs. An advantage of spatially resolved exposure models is that they are a departure from the deterministic approach and can account for spatial variability in model parameters and provide concentration distributions based on this variability (Burns et al., 2021, 2022; McDonough et al., 2022). This can be important across European countries, which can have differences in geographic, population, and wastewater treatment characteristics. Furthermore, a key feature of risk assessment is to apply a tiered approach where lower tier assessments are made with fewer data and conservative assumptions, and higher tiers incorporate more data and realism. Higher-tier assessments can also move beyond deterministically calculated exposure estimates by accounting for variability in exposure parameters (Csiszar et al., 2016; Embry et al., 2014; Flinders et al., 2025; Hollander et al., 2011). Within the context of EU regulatory frameworks (ECHA, 2019), spatially referenced models provide higher-tier exposure estimates for receiving surface waters compared to box models, noting that EU framework models also take into account other environmental compartments.

The detailed model framework is described in McDonough et al. (2022) and is based on geospatial inputs on population, per capita wastewater flow, WWTP locations and infrastructure, and river flow, hydrology, and connectivity, with a focus on data availability, resolution, and accuracy. Publicly accessible, globally consistent datasets were prioritized to ensure transparency and standardization across regions. Following this paradigm, for the European expansion, several data sources were available directly from official EU datasets (EEA, 2021; Eurostat, 2025) and from those leveraged from the global framework (McDonough et al., 2022; Vamshi et al., 2025). The model was demonstrated for several common ingredients used in cleaning and personal care products with down-the-drain disposal routes. Monitored river water concentrations were collected for these ingredients with a focus on spatial coverage across Europe to use a comparison to modeled values for evaluation. Furthermore, the PECs were combined with previously determined predicted no-effect concentrations (PNECs) to demonstrate how the modeled PECs can be applied and interpreted for aquatic safety assessments within a tiered risk assessment approach.

The model described in this article is publicly available and free to use via the iSTREEM web platform (www.istreem.org) with a user interface that takes chemical-specific inputs on wastewater treatment removals, in-stream decay rate, and emissions. The framework incorporates advancements in wastewater treatment representation, in-stream chemical decay, and downstream routing of concentrations, features that enhance its capability to address complex exposure scenarios. By adapting the iSTREEM global model framework to European conditions, this study aims to support technically robust decision-making in chemical management and risk assessment and can be used to complement existing tools (ECHA, 2016; Salvito et al., 2002) to refine exposure assessments following a tiered approach.

Materials and methods

Model framework

The detailed model framework is described in McDonough et al. (2022). Briefly, the model is based on geospatial inputs on population, per capita wastewater generation or water use, WWTP locations and infrastructure, and river flow, hydrology, and connectivity. High spatial resolution was essential to accurately link wastewater discharges to receiving river flows, supporting the model's predictive capability for in-stream chemical concentrations.

The model calculates substance concentrations at emission points using information on emissions, population, per capita wastewater generation, wastewater treatment removal fractions, WWTP discharge flows, and river flows, following the standard risk assessment PEC equation as described in Kapo et al. (2016) and Vamshi et al. (2025). River catchments receive emissions from either WWTPs, or other discharge types, e.g., direct discharge, or from other treatment types. Additionally, the model accounts for in-stream decay as the emissions flow down the river catchments and the chemical is then routed to downstream rivers as additional inputs to the emissions, allowing for chemical connectivity across the river network (Kapo et al., 2016; McDonough et al., 2022). The river routing information for chemical connectivity was provided by the flow dataset of Vamshi et al. (2025), in which river flows are processed at the Level-12 (L-12) HydroBASINS catchment scale (Lehner & Grill, 2013), which serves as the core spatial analysis unit of the model. As such, in addition to the river flows, the values needed as background model input were spatially allocated to each L-12 river catchment. Level-12 catchments are the smallest-sized sub-basin boundaries in the HydroBASINS dataset, where the largest scale (Level-0) refers to continental-level basins (Lehner 2014; Vamshi et al., 2025).

Chemical emissions are typically available on a European level (ECHA, 2016; HERA, 2005; Price et al., 2010; Spaniol et al., 2021); as such, they are spatially allocated in the model based on spatial population distributions. WorldPop (2018) provides a globally available, high-resolution dataset that can be utilized for population inputs and follows the framework of McDonough et al. (2022). For other model inputs (water use and wastewater treatment types), the framework integrates publicly available data, primarily from official EU sources such as the Eurostat and Waterbase databases (EEA, 2021; Eurostat, 2025) and country-specific government databases, to fill data gaps. Wastewater infrastructure accounts for various treatment scenarios, including WWTPs, other treatment types, and direct discharge also from Eurostat databases. Table 1 provides a summary of datasets used to parameterize the model, with population, WWTP locations, and river flows processed at the river catchment scale and per capita wastewater generation processed at the country level.

User inputs to the model include chemical emissions (on a per capita basis), wastewater treatment removal for different scenarios (secondary treatment, other treatment, direct discharge), and in-stream decay rates. Model inputs are externally derived by the user, thus allowing for no limitations on the domain of applicability based on individual chemical properties. The model for Europe includes all EU Member States as well as the United Kingdom, Norway, and Switzerland for a total of 30 countries/states (see online supplementary material for the full list).

Table 1. Summary of all data sources used to parameterize the model following the McDonough et al. (2022) framework.

Model parameter	Description	Source
Population	Processed to Level-12 river catchments	WorldPop (2018) Waterbase PE (EEA, 2021) Eurostat env_ww_con (2023)
Per capita wastewater flow or water use	Country/European Union Member State specific	Eurostat env_ww_genv (2022a) Eurostat env_wat_cat (2022 b) Ireland CSO (2020)
Wastewater treatment infrastructure	Accounts for three treatment scenarios: WWTP with secondary treatment, primary or other treatment, direct discharge. Processed to Level-12 river catchments	Eurostat env_ww_con (2023)
River flow and routing	Processed to Level-12 catchments and flow routed between catchments	Vamshi et al. (2025)
Chemical routing	Leverages iSTREEM and ROUT algorithms	Wang et al. (2005) Kapo et al. (2016)

Note. WWTP = waste water treatment plant; iSTREEM (Kapo et al. 2016) and ROUT (Wang et al. 2005) are names of computer models.

Hydrology and river flow

Characterizing hydrology and river flow is essential for calculating aquatic exposure concentrations, and a spatially connected network of catchments and rivers covering all European countries is needed to parameterize the model. The global river flow dataset of Vamshi et al. (2025) was leveraged in this model, which also includes an algorithm that was created to route flow between catchments. Briefly, this dataset is based on estimating mean annual river flows by leveraging high-resolution spatial data and flow estimation techniques following the curve number approach (USDA, 1986). The estimated flows were combined with hydrological river network and catchment datasets, HydroBASINS and HydroSHEDS (Lehner & Grill, 2013), to connect and route the estimated flows. The approach generated estimates of mean annual flow rates (m^3/s) on the L-12 catchment scale that aligned closely with measured discharges at monitoring gauges, which were available as mean annual discharges (GRDC, 2020). Level-12 catchments are the smallest-sized sub-basin boundaries in the HydroBASINS dataset, where the largest scale (Level-0) refers to continental-level basins (Lehner, 2014; Vamshi et al., 2025). The model was evaluated across several global geographies by comparing to measured gauge river flow data, resulting in good agreement in estimated flows with $R^2 > 0.7$. Additionally, the flows in the three European countries evaluated, France, Germany, and the United Kingdom, were consistent with observed data and tended to be slightly conservative, with estimates generally lower than the observed flows. Further details can be found in Vamshi et al. (2025). As discussed in Vamshi et al. (2025), river flows can have temporal variability, e.g., higher flows during seasons with heavier rainfall and lower flows during lower rainfall, and mean annual flow data were leveraged to represent average yearly conditions for use in risk assessment frameworks.

Per capita wastewater generation

A key parameter for estimating effluent flows from WWTPs is the annual per capita wastewater flow (PCWW), which is combined with the population served by the treatment plant to determine total effluent flow (ECHA, 2016). European PCWW data were primarily sourced from the EU Eurostat database on household wastewater generation (Eurostat, 2022a), where available, and supplemented by country-specific household water use sources when necessary (CSO, 2020; Eurostat, 2022b) (see online supplementary material Table S1). The Eurostat dataset on the generation and discharge of wastewater (env_ww_gen dataset, Eurostat, 2022a) provided the closest approximation to the volume of household wastewater to which chemicals are discharged. The most recent data for domestic wastewater volume were used for each country, and per-capita water volumes were calculated using corresponding population demographic data from the Eurostat database (demo_gind dataset; Eurostat, 2022c).

For countries where wastewater generation data were unavailable, water use data by supply category (env_wat_cat dataset; Eurostat, 2022b), filtered for household usage, were used. As with the wastewater data, household water use volumes were converted to per capita values using population demographics from the same Eurostat dataset (demo_gind dataset) following the summary statistics provided by Eurostat (Eurostat, 2024).

Wastewater and water use data were available from Eurostat databases for all European countries in the model, except Ireland. For Ireland, data on average household water supply and the average number of residents per household were obtained from the Ireland Central Statistics Office (CSO, 2020, 2024). Per capita water use for Ireland was then calculated by dividing household water use by the average number of residents per household, resulting in values comparable to those from other European countries in the Eurostat database (see online supplementary material Table S2). It should be noted that there are combined sewer systems in Europe (Perry et al., 2024), which could result in combined sewer overflows (CSOs) during heavy rainfall events. These were considered currently out of scope for the model and could be an area of future research, which can also help understand the impacts of improving wastewater treatment infrastructure.

Wastewater treatment infrastructure

The European Environmental Agency via the Waterbase-Urban Waste Water Treatment Directive (UWWTD) database provides geographic information system locations of WWTPs across Europe (EEA, 2021). The Waterbase WWTP locations for the 30 countries included in this model were spatially assigned to their corresponding L-12 river catchment from the global river flow network (Vamshi et al., 2025), resulting in each WWTP being linked to the hydrologic river network. Additional processing

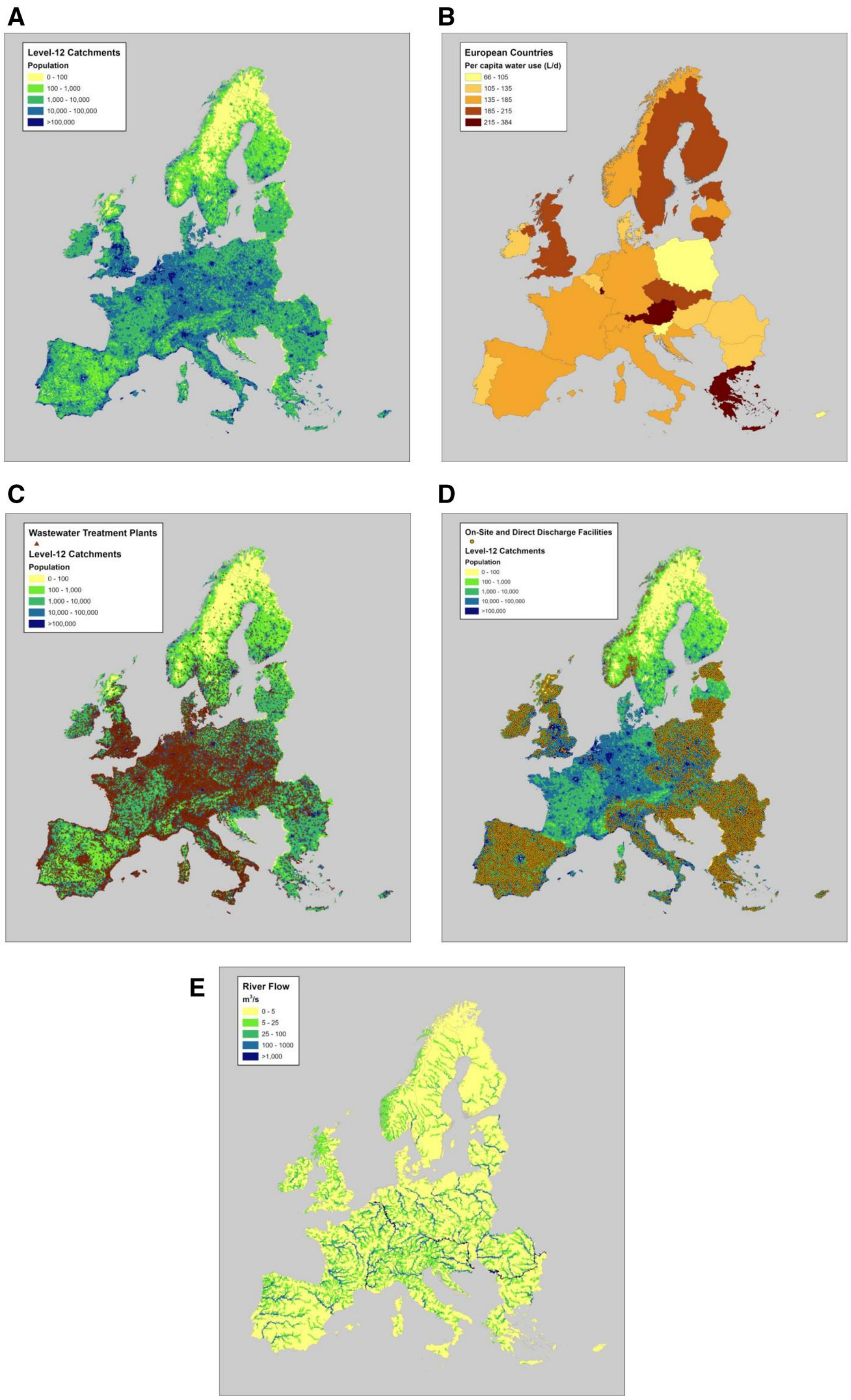

Figure 1. Spatially resolved data inputs for the Europe model processed to river catchments: (A) population, (B) per capita wastewater flow, (C) wastewater treatment plant (WWTP) locations, (D) other treatment and direct discharge locations, (E) river mean annual flow. Note in (C): areas with high density of red circles indicate locations with high density of WWTP sites.

steps, such as ensuring the WWTP was currently active and connected to treatment, were conducted, resulting in 23,952 WWTPs included in the model (Figure 1A) across 13,536 river segments with further details in online supplementary material Section S1.

Within Europe, WWTPs that employ secondary wastewater treatment are the predominant treatment facility type (WISE Freshwater, 2025) and are required under the European UWWTD for WWTPs with population equivalents (PEs) above 1,000 (European Parliament, 2024). Secondary treatment is defined by the UWWTD as a wastewater treatment process that involves biological treatment and a secondary settlement process (European Parliament, 2024). Secondary wastewater treatment facilities are further described to consist of the following processes (in order): a primary settler, an aeration tank (with activated sludge and biological treatment), and a liquids–solids separator, following EU environmental safety assessment guidance (ECHA, 2016; Struijs, 1996). As such, secondary treatment refers to substances undergoing removal via both a primary settling process as well as biological treatment with a secondary settlement process. The finding that WWTPs are dominated by secondary treatment facilities was also found for other model regions such as China and Japan (McDonough et al., 2022), and following the framework, the WWTP locations in the model represent facilities where wastewater influent undergoes the entire secondary treatment process as described in EU technical guidance (ECHA, 2016). Wastewater treatment removal for substances can be calculated using models such as SimpleTreat (Struijs, 2014), quantified in flow-through WWTP simulation studies (e.g., OECD 303A, 2001), measured directly at WWTPs (McAvoy et al., 1998), or calculated from monitoring data (McDonough et al., 2016; Menzies et al., 2019); use of these values for model input follows risk assessment tiered approaches. Modeled removal values also follow a tiered process where modeled chemical property input values can be used at the lower tier, with increasing realism using laboratory input data, for example, applying a default biodegradation rate based on screening study results (e.g. OECD 301, 310, 302 series, 1992a, b, 2014) or measured rates in higher-tier simulation laboratory studies (e.g., OECD 314, 2008) (ECHA, 2019).

The EU Eurostat database provides population-based wastewater treatment infrastructure and connectivity information for individual European countries (Eurostat, 2023). According to a summary of these data (Eurostat, 2024; WISE Freshwater, 2024), greater than 80% of the EU population is connected to at least a secondary WWTP facility, as described above. This leaves 20% of the population with either direct discharge or treatment other than secondary WWTP treatment. The global model framework of McDonough et al. (2022) accounts for populations with treatment types other than secondary treatment and direct discharge by assigning the remaining catchments to have inputs from both direct discharge and other treatment types. Following the framework, this process was also used for the European model and results in three different treatment removal options as model inputs. Within Europe, primary treatment of wastewater is also used (WISE Freshwater, 2025), defined by UWWTD and the European Environment Agency (EEA, 2000; European Parliament, 2024) as a physical or chemical process that reduces biological oxygen demand and suspended solids of incoming wastewater and involves the removal of floating and suspended solids. As such, the other treatment type option in the model input can be used to represent primary treatment in the European version of the model.

Population and emissions

After determining treatment type locations, populations were allocated to each river segment, to be combined with country-specific PCWW to calculate daily wastewater discharge for each catchment. Populations were allocated to each catchment based on three different sources: the WorldPop database (2018) which provides populations across the globe on a 100 × 100 m resolution, PEs associated with each WWTP from the Waterbase dataset (EEA, 2021), and Eurostat information on populations connected to wastewater treatment types on a country level (i.e., secondary treatment, other treatment, and direct discharge) (Eurostat, 2023). All these sources were needed to derive representative information on populations for each river catchment, with further details in online supplementary material Section S1. As these sources provide information on both the catchment and country level, they were combined to arrive at representative populations and associated treatment types for each river catchment. To review resulting values used in the model, river catchment populations were summed for each country and compared to country populations from Eurostat (2022c) and country-level wastewater treatment statistics (Eurostat, 2023).

Populations for each catchment are also used to spatially allocate model input emissions in grams/capita/day (g/c/d) by multiplying catchment populations by the per capita emission provided by the user, following the framework of McDonough et al. (2022).

Model demonstration and case studies

To understand the impacts of model input parameters, a sensitivity analysis was conducted by altering each key input parameter independently at a constant emission (1 g/c/d) and comparing differences to the 50th percentile concentration following the framework of McDonough et al. (2022). The model was demonstrated and further evaluated using case studies for chemicals used in household down-the-drain applications and spanning a range of model input parameters. These include linear alkylbenzene sulfonate (LAS) (C10-13 chain length (C10-13 LAS)) and alkyl sulfate (AS) (C12 chain length (C12-AS)), which are both surfactants with LAS commonly used in laundry detergents and AS commonly used in both laundry detergents and personal care products (HERA, 2002, 2013; Spaniol et al., 2021); and oxybenzone (CAS: 131-57-7) and octinoxate (CAS: 5466-77-3, 83834-59-7), which are ultraviolet (UV)-filters used in personal care products (Burns et al., 2021, 2022). For LAS and AS, the chain lengths were chosen to reflect the most used chain lengths, which enabled both the collection of emissions and monitoring data for model comparison (HERA, 2013; Spaniol et al., 2021). Model inputs on emissions, wastewater treatment removal, and in-stream decay are summarized in the results section. Yearly per capita emissions were derived from recently reported yearly emissions (kg/y) for each ingredient C10-13 LAS (Greiner et al., 2021; HERA, 2013), C12-AS (Spaniol et al., 2021), and oxybenzone and octinoxate (Euromonitor, 2021) and scaled to populations of countries included in the respective estimates. For LAS and AS, secondary WWTP removal percentages were sourced from previously conducted safety assessments in Europe and were based on measured removals at WWTPs (HERA, 2002, 2013). For the UV-filters, secondary WWTP removal percentages were derived from data reported by Burns et al. (2021, 2022) and also based on measured WWTP removals. As discussed previously, the "other treatment" model input can be represented by primary removal. For the surfactants, primary removals were sourced from previous assessments (HERA, 2002, 2013) using sorption to sludge as a proxy for primary removal; however, it should be noted that WWTP removal for these surfactants has been found to be mainly via biodegradation (ECHA, 2017, 2024). For the UV-filters, primary removals were estimated using the SimpleTreat 4.0 model (Struijs, 2014) using physical–chemical property and biodegradation data as inputs from Burns et al. (2021, 2022) (details for all substances in online supplementary material Section S2 and Table S3). For LAS and AS, McDonough et al. (2016) reported measured values of in-stream decay with half-lives of 0.35 and 0.08 days, respectively, indicating that these materials continue to undergo rapid biodegradation in river waters. These measured decay rates were leveraged as model inputs following EU technical guidance (ECHA, 2016, 2019) (details in online supplementary material), which indicates decay rates should reflect water temperatures of 12°C; however, it should be noted that this may be a conservative assumption and could be refined to reflect more realistic scenarios. For the UV-filters, European default values for readily biodegradable (octinoxate) and readily biodegradable-not meeting the 10-day window were used (oxybenzone) following Burns et al. (2021, 2022) and EU technical guidance (ECHA, 2016).

All case study substances have extensive surface water monitoring data in European rivers which were collected from several sources including the literature (Briels et al., 2023; Burns et al., 2021, 2022; Chiriac et al., 2021; Finckh et al., 2024; Freeling et al., 2019; Malnes et al., 2022) and monitoring databases such as the European NORMAN (2024) database and the European Environmental Agency Waterbase Water Quality database (EEA, 2024) to use as comparison between modeled and measured concentrations, with focus on spatial representation across Europe. To capture spatial variability in monitored concentrations based on yearly consumer use, when there were data from the same location at differing times, these were averaged to represent a single entry for a given location. This ensures that resulting distributions represent spatial variability and were not skewed toward single locations with more sampling time points (further data processing steps and details in online supplementary material Section S3 and Table S4). Parameters indicative of data quality and relevance (e.g., limit of detection, sample size) were considered in data curation and discussed in online supplementary material Section S3, although a standardized assessment scheme such as CREED (Merrington et al., 2024) was not used.

The model provides estimated concentrations at the start of river segments containing WWTP facilities (13,536 segments). These segments were selected due to the uncertainty in direct discharge and other treatment type locations. The concentrations at the beginning of each segment represent estimates at the WWTP facility mixing zone, providing the most conservative values for a river segment. This approach accounts for all upstream background inputs in addition to discharges from the treatment plant. River segments without WWTP facilities were still routed through each segment and included as background concentrations, aligning with other European exposure modeling frameworks (ECHA, 2016). To minimize errors in probabilistic distributions, particularly at the extremes, modeled concentration distributions were evaluated from the 10th to 90th percentiles, ensuring robustness when integrating large datasets from multiple sources (McDonough et al., 2022).

The case studies were also used to demonstrate how the modeled concentration distributions can be used as PECs in aquatic risk assessment following the framework in Burns et al. (2022) and using previously derived PNECs for all materials (Burns et al., 2021, 2022; ECHA, 2017, 2024; HERA, 2013) compliant with European regulatory guidance.

Table 2. Summary of model background data across all countries in the model.

Population	530 million
Per capita wastewater flow	162 L/c/d (population weighted average)
Number wastewater treatment plants (WWTPs)	23952
Population connected to secondary treatment	83%
Population with other treatment	8%
Population with direct discharge	9%
Population with some form of wastewater treatment	92%

Note. L/c/d = liters/capita/day. The population with wastewater treatment (last row) represents the sum of populations connected to secondary and other treatment types.

Results and discussion

Model background data summary

Maps of the spatial distribution of population, WWTP locations, other treatment/direct discharge locations, PCWW, and river flow can be found in Figure 1. The model summary values of population, PCWW, number of WWTPs, and percentage of population connected to wastewater treatment types are in Table 2 and summarized on a country level in online supplementary material Table S2.

For the population processing, as an initial comparison on a country level, the sum of the population treated at WWTPs (Waterbase PE; EEA, 2021) was compared to the sum of populations from the WorldPop (WP) database (WorldPop, 2018), following the same validation methods as described in McDonough et al. (2022). The results of the comparison indicated that for some countries, the sum of the PE was higher than the country population, and in other cases did not yield a percentage of population served consistent with those reported by the EU Eurostat database (Eurostat, 2023). To address this inconsistency, for catchments with WWTPs, catchment-specific PE values from Waterbase were adjusted with a country-specific constant fraction to ensure that when compared on a country level that the population connected to secondary WWTPs was consistent with values reported by Eurostat (Eurostat, 2023) (see online supplementary material Table S2). Similarly, for river catchments that did not have WWTPs located on them (other treatment and direct discharge), the WP populations were scaled to country-specific values based on the remaining population needed for each country after accounting for populations with secondary wastewater treatment. The resulting model population is 530 million, which was relatively evenly distributed across the continent, except for lower populations in the northern parts of Norway, Sweden, and Finland (Figure 1A). Each country population in the model (which was calculated on a country level by summing populations associated with each catchment that fall within a given country) was compared to country-level populations reported by Eurostat (Eurostat, 2025), and all populations were consistent (online supplementary material Figure S1).

The PCWW ranged from 82 to 383 L/c/d with a population weighted average of 162 L/c/d. This is comparable to but lower than the value used in the EU technical guidance of 200 L/c/d parameterization (ECHA, 2016) based on values from the SimpleTreat 3.0 model (Struijs, 1996). The results are also comparable to the average wastewater production of 157–251 L/c/d (57.9–91.7 $m^3/c/y$) reported by Jones et al. (2021) for Eastern Europe & Central Asia and Western Europe, respectively. While the values used in this model are comparable to but lower than other values in the literature, they represent domestic wastewater generation as reported by the EU Statistics office (Eurostat, 2022a) and were considered the best available for inclusion in the model. There is a relatively large range of PCWW across Europe (Figure 1B) based on country-specific water infrastructure; however, the median value across the countries was 158 L/c/d.

In total, the number of WWTPs in the model is 23,952, noting in general, the location of the treatment plants generally occurs where there is a higher population (Figure 1). The overall population connected to at least secondary treatment is 83% and consistent with data summarized by the EU statistics office, as more than half of the Member States having 80% or greater connectivity to at least secondary treatment (Eurostat, 2024). The population connected to other treatment types (e.g., primary treatment) was 8%, leaving 9% of the population with direct discharge. Thus, the population connected to some form of wastewater treatment is 92%, with the range across countries of 57%–100%, with 93% of the countries having treatment levels of 78% or greater.

River flows varied across the continent, with the larger flows primarily in the mid- to northern mainland regions. The lower flows were as expected, in the more southern regions where there are drier climates and in the northern regions, likely due to higher snow cover (Vamshi et al., 2025).

Sensitivity analysis

The model was evaluated by varying user input parameters individually to understand the impacts of changing parameters on model results. As such, percent removal during the various treatment types, as well as in-stream decay, were varied, with a default emission of 1 g/c/d, and 50th percentile concentrations were used for illustrative purposes (see online supplementary material Figure S2). For the entire model, when varying removal rates individually, as the population connected to secondary treatment is relatively high (83%), increasing secondary treatment removal has the largest impact on reducing river concentrations compared to varying other treatment types individually. However, as expected, if all treatment types are varied together, then this has the largest impact on reducing river concentrations. For example, the reduction in river concentrations from 0%–90% treatment is a factor of 6 when increasing secondary treatment only; however, the reduction is a factor of 10 when all treatment types are included (see online supplementary material Figure S2). This indicates that increasing removals in areas where there are only direct discharge or other treatment types could have an impact on reducing concentrations across the continent. Additionally, as expected, as emissions are higher in areas with higher populations, concentrations were also higher for segments with higher populations associated with them compared to those with lower populations (see online supplementary material Figure S2). For the entire model, varying in-stream decay rates indicates that there is a sharp reduction in concentrations even at a rate of 0.35 d^{-1} (two times reduction) and can be reduced by a factor of ~3 if the decay rate is 4 d^{-1} or faster. Once the decay rate reaches 4 d^{-1}, the concentration plateaus, indicating that at this decay rate, maximum decay occurs in the given catchment river transit time. McDonough et al. (2016) have reported surfactant in-stream decay rates (due to biodegradation) ranging from 2 to 8.5 d^{-1}, indicating that this is an important factor to consider for biodegradable compounds. The sensitivity analysis provides confidence that the model results are consistent with expected results, that is, increasing wastewater removal rates and in-stream decay rates reduced concentrations. The analysis provided further insights into how wastewater treatment infrastructure and continued biodegradation under environmental conditions across the various countries can influence river concentrations.

Case study exposure assessment

The model inputs for the case study substances (C10-13 LAS, C12 AS, oxybenzone, octinoxate) are summarized in Table 3. Maps of modeled concentrations across the river segments are in online supplementary material Figure S3 for all case study substances. Consistent with the sensitivity analysis, concentrations were generally higher in more populous areas. The model was designed to predict exposure distributions accounting for spatial variability; however, it was not designed or evaluated for location-specific assessment. As such, model evaluation was performed by comparing monitored and modeled concentration distributions. As the main application of this model is to understand concentration distributions across Europe for application in risk assessment, modeled concentrations are represented as distributions representing spatial variability in exposure estimates across the river segments (Figure 2). Details of the processing of monitoring data for comparison to modeled data are in online supplementary material Section S3, resulting in over 100 unique monitored values for each material across ≥ 11 countries; these were also converted into concentration distributions for comparison to measured data. Modeled and monitored values were compared using percentiles from the concentration distributions, which allows for a comparison not only of the magnitude of the values, but also spatial distribution (McDonough et al., 2022). All the substances had several nondetect (ND) or lower than quantification (LOQ) values (37%–73%, Table 3), and these were set to half the ND/LOQ values for data processing. For the C10-13 LAS and oxybenzone case studies, there were enough detected values (63% and 40%, respectively) to enable comparison of the spatial distribution by plotting measured and monitored percentile concentrations (McDonough et al., 2022) to additionally evaluate model performance. These plots represent modeled versus monitored concentration percentiles across a range of percentiles from their respective concentration distributions (e.g., 50th percentile modeled concentration versus 50th percentile monitored concentration) (Figure 3).

For C10-13 LAS surfactant, there were 160 values (representing unique locations) in the resulting monitoring dataset across 11 countries, with 37% ND values (Table 3). As the detection frequency is greater than 50%, median, 75th percentile and 90th percentile concentrations were used for comparison. Monitored concentrations across these percentiles were 1, 5, and 10 μg/L, respectively, with modeled concentrations of 2, 6, and 20 μg/L, respectively, indicating the model was within a factor of 2 and

Table 3. Model input parameters for case study substances and summary of monitoring data used for comparison.

	C10-13 LAS	C12 AS	Oxybenzone	Octinoxate
Emission (g/c/d)	2.8	0.7	0.002	0.006
Secondary treatment removal (%)	99	99	86	96
Primary treatment removal (%)	20	3	5.4	43
In-stream decay (d^1)	1.0	4.6	0.014	0.046
Monitoring data summary				
Number data points:	$n = 160$	$n = 131$	$n = 200$	$n = 443$
ND/LOQ frequency:	ND/LOQ: 37%	ND/LOQ: 73%	ND/LOQ: 60%	ND/LOQ: 70%
Number countries:	Countries: 11	Countries: 11	Countries: 19	Countries: 18

Note. AS = alkyl sulfate; g/c/d = grams/capita/day; LAS = linear alkylbenzene sulfonate; n = number; ND/LOQ frequency refers to the percent of monitoring data that were below the ND (nondetect) or LOQ (limit of quantification). References and derivation details are described in the main text and online supplementary material Section S3.

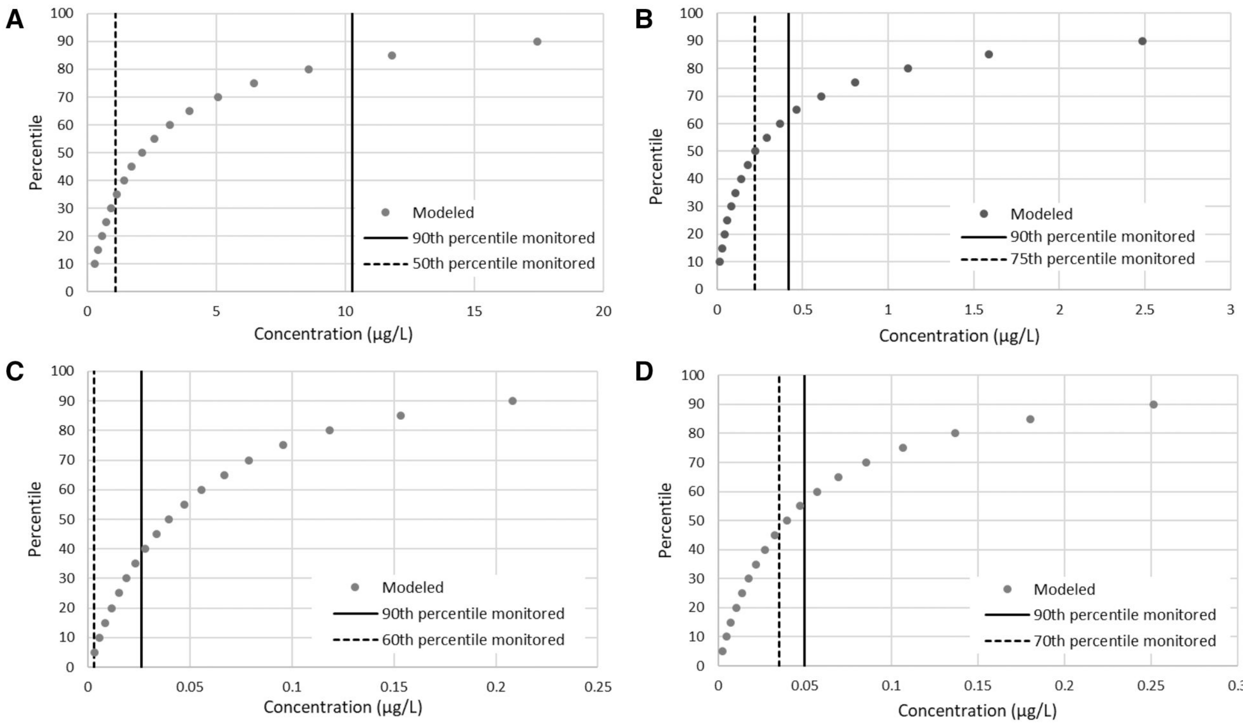

Figure 2. Modeled concentration percentile distributions with straight lines indicating monitoring data percentiles for (A) C10-13 LAS (linear alkylbenzene sulfonate), (B) C12 AS (alkyl sulfate), (C) oxybenzone, and (D) octinoxate.

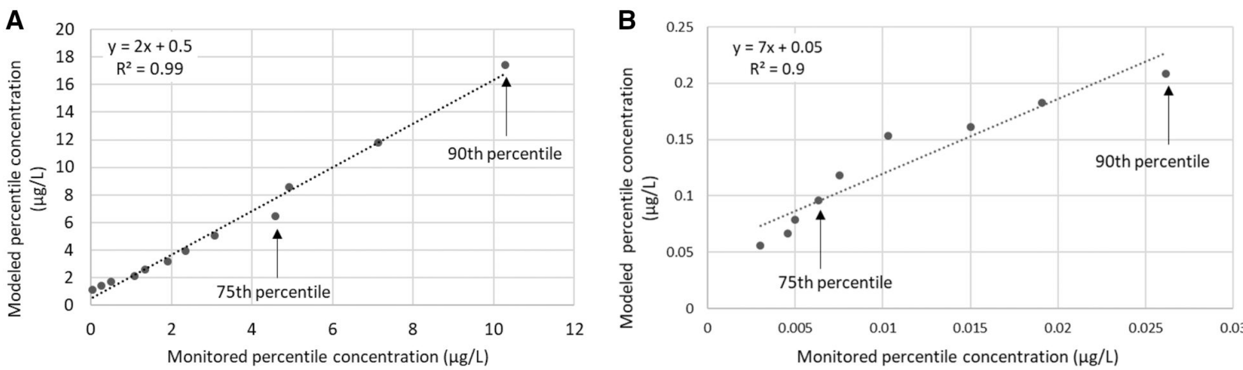

Figure 3. Modeled versus monitored concentration percentiles across (A) 35th–90th percentiles for C10-13 LAS (linear alkylbenzene sulfonate) and (B) 60th–90th percentiles for oxybenzone. The dotted line indicates the linear fit.

consistently conservatively overpredicted (Figure 2A). Comparing concentrations above the ND levels (35th–90th percentiles) by plotting modeled versus percentile concentrations indicated very good agreement ($R^2 = 0.99$) and on average an overestimation of a factor ∼2 (Figure 3A).

For C12 AS surfactant, the analysis resulted in 131 monitored values across 11 countries with 73% ND values (Table 3), indicating that the detection frequency for this surfactant was only 27%. As such, comparison was limited to the 75th and 90th percentile concentrations. Monitored concentrations across these percentiles were 0.2 and 0.4 μg/L, respectively, with modeled concentrations of 0.8 and 2.5 μg/L, respectively, indicating the model was within a factor of ∼6 and conservatively overpredicted (Figure 2C).

For oxybenzone (UV-filter), the analysis resulted in 200 monitored values across 19 countries with 60% ND values (Table 3). With a detection frequency of 60%, 60th and 90th percentile concentrations were used for comparison. Monitored concentrations across these percentiles were 0.003 and 0.02 μg/L, respectively, with modeled concentrations of 0.07 and 0.2 μg/L, respectively, indicating the model was within an order of magnitude and consistently conservatively overpredicted (Figure 2C). Comparing modeled versus monitored concentrations by plotting across the 60th–90th percentile concentrations indicated good agreement ($R^2 = 0.92$) and on average an overestimation of a factor ∼7 (Figure 3B).

For octinoxate (UV-filter), the analysis resulted in 443 monitored values across 18 countries with 70% ND values (Table 3), indicating that the detection frequency for this UV-filter was only 30%. As such, comparison was limited to the 70th and 90th percentile concentrations. Monitored concentrations across these percentiles were 0.04 and 0.05 μg/L, respectively, with modeled concentrations of 0.1 and 0.25 μg/L, respectively, indicating the model was within a factor of ~5 and conservatively overpredicted (Figure 2D).

For all case studies, it was found that the model was predictive while still being conservative (i.e., overestimating) when compared to monitoring data. While the model demonstrates how concentrations can be further understood by introducing environmental realism and variability in background parameters, there are several factors that may have contributed to modeled concentrations being overestimated and provide opportunities for future refinements. For example, for C12 AS, Menzies et al. (2017) reported that it can undergo rapid biodegradation in sewers with a measured in-sewer biodegradation rate of 41 h^{-1} following an OECD 314A guideline study (OECD, 2008). This indicates that sewer removal could be a significant loss process, thereby reducing emissions to WWTPs and subsequent environmental concentrations in receiving waters. For LAS, on the other hand, Menzies et al. (2017) reported minimal in-sewer decay in an OECD 314A study, indicating that this may not be a significant loss process for LAS. This could explain the difference in the higher overprediction of AS concentrations compared to LAS in this study, when compared to monitoring data.

Another key environmental loss process for biodegradable compounds is continued in-stream biodegradation as captured in the model. European Union modeling guidance (ECHA, 2016) assumes that European river waters are on average at a temperature of 12 °C, and measured in-stream decay rates for the surfactants (McDonough et al., 2016) were converted to this temperature to be consistent with the guidance. However, this could be a conservative assumption, and in-stream decay may be occurring at warmer temperatures, which could have also contributed to the conservatism of the predictions. For the UV-filters, in lieu of measured in-stream decay rates, EU guidance conservative default values also at the default temperature (ECHA, 2016) were used; however, as can be seen with the surfactants, higher-tier measured values could yield faster in-stream decay rates. As such, these assumptions could have also led to overpredicted concentrations. Other in-stream loss processes, such as volatilization, suspended sediment partitioning, and abiotic degradation, were also not accounted for and could provide further avenues for refinement.

Another factor contributing to the UV-filters being overpredicted is having fewer measured data available for parameter refinements (e.g., in-stream decay rates), and another assumption was that the emission estimates conservatively assumed that all the personal care products containing the UV-filters were disposed down-the-drain. However, UV-filters are also used in primary sunscreen products with direct emissions to water bodies (oceans, lakes) via swimming, e.g., and as such, emissions used are likely higher than those going down-the-drain into receiving rivers (Burns et al., 2021, 2022). While there may also be seasonality in the use of UV-filter products, e.g., higher use in summer months, this pattern was not observed in WWTP monitoring campaigns for both oxybenzone and octinoxate (Burns et al., 2021, 2022) and likely does not affect the modeling results, which represent daily product use over a year. If further information on allocation of ingredient volumes to daily personal care products (e.g., facial care) versus primary sunscreens becomes available, concentrations can be further refined (Burns et al., 2021, 2022).

Also noteworthy is that all the substances had substantial ND values in the monitoring datasets (37%–73%) which also results in model predictions being higher than monitored values. The large amount of the ND values also provide further indications that there can be further refinements, as described above, and that additional loss mechanisms are likely occurring under environmental conditions or other refinements could be made. Furthermore, while the monitoring datasets include greater than 100 unique monitored sites for each compound, there may still be uncertainty in these values as well.

Application to risk assessment

In this section, the application of the model in a risk assessment framework is demonstrated for the four case study materials following the framework of Burns et al. (2021). The focus of this analysis is to demonstrate a risk assessment evaluation by comparing PECs (i.e., modeled percentile concentration estimates) to PNECs, where PECs below PNECs are considered low or negligible risk (ECHA, 2016). The exposure assessment is then put into a tiered context with additional comparison of monitored concentration percentiles to PNECs. When PECs are below the PNEC, no ecological effects are predicted to occur to aquatic organisms. Robust PNECs that have been previously derived, based on acute and chronic data across at least three trophic levels, were leveraged in these assessments (Burns et al., 2021, 2022; ECHA, 2017, 2024; HERA, 2013), and follow the European PNEC derivation guidance (ECHA, 2008) (Table 4).

Table 4 summarizes 25th–90th percentile modeled and monitored concentrations (PECs) for C10-13 LAS, C12 AS, oxybenzone, and octinoxate. The median modeled PECs are at least 1–2 orders of magnitude lower than the PNEC for all substances. The 90th percentile modeled PECs, considered a reasonable worst-case scenario in risk assessment frameworks (ECHA, 2016; Nabholz, 1991), are all also substantially lower than their respective PNEC for all substances. Modeled concentration distributions across Europe are well below each PNEC, suggesting that adverse effects in freshwater environments from these chemicals are unlikely.

Table 4. Summary of measured and modeled percentile predicted environmental concentrations PECs for C10-13 LAS, and C12 AS, octinoxate, oxybenzone, and PNECs for use in risk characterization.

PEC percentile (μg/L)	C10-13 LAS		C12 AS		Oxybenzone		Octinoxate	
	Monitored	Modeled	Monitored	Modeled	Monitored	Modeled	Monitored	Modeled
90th	10	20	0.4	2.5	0.03	0.2	0.05	0.25
75th	4.6	6	0.2	0.8	0.006	0.1	0.04	0.2
50th	1	2	ND	0.2	ND	0.04	ND	0.04
25th	ND	0.7	ND	0.06	ND	0.02	ND	0.01
PNEC (μg/L)	268		176		18		1	
PNEC source	HERA (2013), ECHA (2024)		ECHA (2017)		Burns et al. (2021)		Burns et al. (2022)	

Note. AS = alkyl sulfate; LAS = linear alkylbenzene sulfonate; PEC = predicted environmental concentration; PNEC = predicted no-effect concentration; ND refers to values were below the ND (nondetect) limit or LOQ (limit of quantification).

As discussed in the previous section, modeled concentrations align well with monitored values, while still being conservative (i.e., overestimated). This result is consistent with a tiered risk assessment approach, whereby modeled exposure estimates should offer a conservative understanding of chemical concentration effects on aquatic environments; however, they can be refined further to incorporate higher-tier data or more environmental realism. Comparing the PNECs to the monitored concentration distributions offers further insights into how much concentrations can be further refined. As a comparison, median monitored PECs for AS, oxybenzone, and octinoxate were all below ND values, and the median monitored PEC for LAS is 2 orders of magnitude lower than the PNEC. Furthermore, 90th percentile monitored PECs were all lower than PNECs by 1–2 orders of magnitude (Table 3) for all compounds. The large amount of ND concentrations across the compounds (37%–73%) provides further indication that adverse effects in freshwater environments from these chemicals are unlikely; they also demonstrate how modeled values could be further refined for the risk characterization. It should also be noted that though the PNECs used are considered sufficiently robust for these case risk assessments, they could still be further refined to more accurately represent environmental hazard potential. Given the conservative nature of lower-tier hazard assessment, this refinement would be expected to further increase the difference between PEC and PNEC, thus providing additional support for the negligible environmental safety risk associated with the release of these chemicals down-the-drain. Additionally, these case studies provide a demonstration of how the modeled concentration distributions can be applied in risk assessment, for example, when refinements for screening level assessments of other substances are prioritized, such as those with differing PNECs or lower availability of fate and exposure properties.

By simulating conservative concentration distributions, the model identifies areas and chemicals needing further investigation or higher-tier methods. This modeling method is valuable in providing predictive, yet conservative exposure estimates when monitored data are scarce, aiding early-stage environmental risk assessments and prioritizing chemicals for further testing and monitoring. The modeled PECs in Table 4 show negligible risk from down-the-drain disposal of these chemicals, making further high-tier environmental fate and toxicity data refinement for WWTP effluent-receiving freshwaters in Europe for these materials a low priority.

The model was designed to fit into a risk assessment framework where substance emissions are generally available on a European level; however, further model refinements could include addressing spatial variability in product usage. For example, Hodges et al. (2014) found population variability in product use across Asia based on gross domestic product. Furthermore, as emissions are also generally available on a yearly basis (tonnage/year), the model does not take temporal variation into account; however, future developments could incorporate this variation. While the model goal was to address spatial variability in background parameters for environmental risk assessment based on yearly emissions and environmental conditions, there can also be temporal or seasonal variability, for example, in river flow rates, which could also be incorporated into future versions. The model has been previously demonstrated to be predictive yet conservative compared to monitoring data for the United States, China, and Japan based on yearly emissions and flow conditions (Burns et al., 2021, 2022; Kapo et al., 2016; McDonough et al. 2022).

Conclusions

This study demonstrates the application of a modeling framework to estimate aquatic chemical concentrations based on spatial variability in model parameters across Europe (EU, Norway, Switzerland, UK) for substances disposed down-the-drain. Spatially referenced exposure models can provide valuable insights into prospective risk assessments where monitored data may be limited or can provide higher-tier exposure estimates beyond deterministic models. This model, which simulates conservative concentration distributions in the absence of direct measurements, can serve as a useful tool for understanding the potential risks of chemical exposure in aquatic environments across various regions.

The study modeled concentrations for substances used in laundry detergents and personal care products across Europe, resulting in predictive yet conservative predictions for all substances that are appropriate for use in a tiered risk assessment process, allowing for further refinements. Comparison of modeled concentration distributions of C10-13 LAS and oxybenzone exhibited good agreement with monitored values ($R^2 = 0.99$ and $R^2 = 0.92$, respectively), demonstrating that the model was able to capture spatial variability. Despite varying detection frequencies, the model's consistency highlights its utility in understanding concentration distributions for tiered risk assessments. As the model requires minimal input data, it also has potential for simulating the fate of difficult-to-test substances and polymers for which obtaining accurate parametrization of the physical–chemical and fate properties can be challenging.

The findings of Kapo et al (2016), McDonough et al. (2022), and Burns et al. (2021, 2022) support the predictive and conservative nature of the model with their results for the United States, China, and Japan versions of the model framework. This expansion to Europe has resulted in consistent results with these applications that reinforce the model's reliability as a predictive and conservative tool for chemical concentration estimates across diverse global regions. Given that emissions data are typically available at a regional or European level rather than at the national level, it is more appropriate to interpret the results on a broader European scale. However, future research could refine the model by developing country-specific frameworks using available background data to provide more localized insights.

Supplementary material

Supplementary material is available online at *Integrated Environmental Assessment and Management*.

Data availability

The model and river flow data used in the model are available at http://www.istreem.org. The remaining data underlying the model were derived from sources in the public domain: Eurostat database (https://ec.europa.eu/eurostat/data/database), European Environment Agency Datahub (https://www.eea.europa.eu/en/datahub), and WorldPop (https://www.worldpop.org/).

Author contributions

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Conflicts of interest

The authors declare that there are no conflicts of interest.

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