The Influence of Contaminants of Emerging Concern on Beneficial Uses of Water

By Larry B. Barber, Jeramy R. Jasmann, Elizabeth J. Tomaszewski, and Barbara A. Bekins

Chapter D of

Knowledge Gaps and Opportunities for Understanding Water-Quality Processes Affecting Water Availability for Beneficial Uses

Edited by Anthony J. Tesoriero, Melinda L. Erickson, Christopher H. Conaway, Elizabeth J. Tomaszewski, and Christopher T. Green

Open-File Report 2023–1086

U.S. Department of the Interior
U.S. Geological Survey

U.S. Geological Survey, Reston, Virginia: 2024

Suggested citation:
Barber, L.B., Jasmann, J.R., Tomaszewski, E.J., and Bekins, B.A., 2024, The influence of contaminants of emerging concern on beneficial uses of water, chap. D *of* Tesoriero, A.J., Erickson, M.L., Conaway, C.H., Tomaszewski, E.J., and Green, C.T., eds., Knowledge gaps and opportunities for understanding water-quality processes affecting water availability for beneficial uses: U.S. Geological Survey Open-File Report 2023–1086, 18 p., https://doi.org/10.3133/ofr20231086.

ISSN 2331-1258 (online)

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Conversion Factors

U.S. customary units to International System of Units

Multiply	By	To obtain
	Length	
mile (mi)	1.609	kilometer (km)
	Volume	
gallon (gal)	3.785	liter (L)
billion gallons (Ggal)	3,785	cubic kilometer (km^3)
	Flow rate	
gallon per day (gal/d)	0.003785	cubic meter per day (m^3/d)
billion gallons per day (Ggal/d)	43.81	cubic meter per second (m^3/s)

International System of Units to U.S. customary units

Multiply	By	To obtain
	Length	
kilometer (km)	0.6214	mile (mi)
	Volume	
liter (L)	0.2642	gallon (gal)
cubic centimeter (cm^3)	0.06102	cubic inch (in^3)
	Flow rate	
cubic kilometer per day (km^3/d)	264.2	billion gallon per day (Ggal/d)
	Mass	
gram (g)	0.03527	ounce, avoirdupois (oz)
kilogram (kg)	2.205	pound avoirdupois (lb)
	Density	
kilogram per liter (kg/L)	8.345	pound per gallon (lb/gal)

Supplemental Information

Concentrations of chemical constituents in water are given in either milligrams per liter (mg/L) or micrograms per liter (µg/L).

Activities for radioactive constituents in water are given in picocuries per liter (pCi/L).

Abbreviations

BPA	bisphenol A
CEC	contaminants of emerging concern
DoD	U.S. Department of Defense
EDC	endocrine disrupting chemical
EDTA	ethylenediaminetetraacetic acid
EPA	U.S. Environmental Protection Agency
GC-MS/MS	gas chromatography tandem mass spectrometry
HAB	harmful algal bloom
ICP-MS	inductively coupled plasma mass spectrometry
IWS	Integrated Water Science
K_{oc}	soil organic carbon partitioning coefficient
K_{ow}	octanol-water partitioning coefficient
LNAPL	light non-aqueous phase liquids
LC-MS	liquid chromatography mass spectrometry
MCL	maximum contaminant level
MTBE	methyl tertiary butyl ether
PAH	polyaromatic hydrocarbon
PCB	polychlorinated biphenyl
PFAS	per- and polyfluoroalkyl substances
PFOA	perfluorooctanoic acid
PFOS	perfluorooctane sulfonic acid
PPCP	pharmaceutical and personal care products
TCA	1,1,1-trichloroethane
TCE	trichloroethylene
TP	transformation product
USGS	U.S. Geological Survey
VOC	volatile organic compounds
WMA	Water Resources Mission Area
WWTP	wastewater treatment plant

Chemical Symbols

As	arsenic
Ba	barium
Cd	cadmium
Cl	chlorine
Cu	copper
Pb	lead
Ra	radium
Sr	strontium
Zn	zinc

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[Also see https://doi.org/10.3133/ofr20231086]

Chapter D

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Purpose and Scope

This chapter is focused on identifying knowledge and data gaps, that if filled, could improve the ability to incorporate, model, and predict the effects of contaminants of emerging concern (CECs) on intended beneficial uses of water. The gaps identified in this chapter are not intended to be comprehensive but are instead focused on key opportunities for the U.S. Geological Survey (USGS) Water Resources Mission Area (WMA, https://www.usgs.gov/mission-areas/water-resources). CEC's effects on ecosystems are not addressed in this chapter but are covered in the companion Open-File Report to this publication (Harvey and others, 2024) in their chapter C "Anthropogenic and Geogenic Contaminant Bioexposures Affecting Aquatic Ecosystems."

Statement of Problem

What is a contaminant of emerging concern (CEC)? There is no single consensus, definition, or static list of CECs (Diamond and Burton, 2021). A CEC list must be dynamic, as new chemicals are continuously developed, produced, and detected with analytical advancements (Murray and others, 2010). The U.S. Department of Defense (DoD) definition includes the criteria: (1) presents a potential human health or environmental risk, and (2) has new or changing toxicity estimates or environmental regulatory standards (DoD, 2019). Based on the criteria, CECs include both new chemicals that little is known about, and legacy chemicals with renewed attention due to new information about occurrence or health effects. For example, in the case of legacy contaminants, new science shows that reactions of legacy pesticide and petroleum hydrocarbons can result in contamination by both the parent compounds and transformation products (Bekins and others, 2016; Mahler and others, 2021). Similarly, per- and polyfluoroalkyl substances (PFAS) have existed for decades but it is only recently that their many pathways to natural waters and their consequent widespread occurrence and potential health risk have been recognized (Ahrens and Bundschuh, 2014; Guelfo and Adamson, 2018; Sunderland and others, 2019; Ankley and others, 2021). In addition, improved analytical detection limits for CECs have led to recognition of more widespread occurrence across the Nation and awareness of the potential risk to environmental and human health caused by chemicals that are biologically active by design (Barber, 2014). Thus, the definition of CECs results in a mix of chemicals that changes with time and understanding (Barber, 2014). Determining the environmental fates and toxic effects of individual CECs can be challenging because they often occur as complex mixtures with complex effects (Kolpin and others, 2002; Barber, 2013; Bradley and others, 2016; Masoner and others, 2019; Battaglin and others, 2020). Treated wastewater is one of the largest sources of water with complex mixtures of CECs. In water-stressed areas there is a growing need for better understanding of the environmental fate and biological effects of CECs for de facto water reuse for drinking water and for sustainable ecosystem health in those streams with high percentages of total flow coming from accumulated wastewater discharge.

We have identified three specific gaps in CEC research and knowledge: (1) wastewater reuse and anthropogenic return flow relationships to water quality, (2) point-source sites and legacy contaminants, and (3) transformation products as CECs. Transformation products (TPs) are molecules formed from the original contaminant by metabolism, biotransformation, and (or) chemical reactions with light and (or) other chemical species. This list is not intended to be comprehensive but rather to highlight opportunities to address gaps in knowledge as they relate to current USGS priorities. We first address the status of knowledge and capabilities in relation to CECs as a class of contaminants. Each of the three gaps is then discussed in detail, with a statement of problem, status of knowledge, and suggested approaches. We conclude with a summary of outcomes for the USGS.

Status of Knowledge and Capabilities

CECs can be considered from a chemical and a microbial perspective (Cozzarelli and others, 1995; Johnson and others, 2002); however, in this document we only address chemical contaminants when discussing CECs. The sources of CECs are as varied as the contaminants themselves, ranging from municipal wastewater to septic tanks to agricultural run-off to chemical spills. Downstream water quality is known to be degraded by treated municipal wastewater discharge (Kolpin and others, 2002;

Barber, 2014; Bradley and others, 2016; Bradley and others, 2017; Gallen and others, 2018; Battaglin and others, 2020), industrial contaminants from wastewater discharge and chemical spills (Squillace and others, 1996; Landmeyer and others, 1998; Akob and others, 2016; Zhang and others, 2016; Cozzarelli and others, 2021), and return flows from agricultural practices (Kolpin and others, 2002; Murray and others, 2010; Salimi and others, 2017; Woodward and others, 2018, 2019). USGS scientists can prioritize investigations into the ever-increasing suites of new CECs, their sources and exposure pathways, and their effects on potential downstream water uses, by focusing on complex mixtures of contaminants coming from predominant source types. Three broad categories of sources related to water use discussed here are: (1) municipal wastewater, (2) industrial waste and products, and (3) agricultural practices and waste (table D1). Within each of these categories are classes of contaminants that have various uses, occurrence, and toxicity. Although new classes of contaminants and new contaminants themselves are always being identified, the examples in the following discussion highlight the wide range of contaminant chemistry that should be considered.

Municipal Wastewater and Return Flows

Wastewaters are a main source of CECs to freshwater environments (Glassmeyer and others, 2005; Fork and others, 2021), with the loads in surface water being more highly characterized compared to the loads in groundwater (Lapworth and others, 2012). A broad class of contaminants ubiquitously found in municipal wastewater effluents is pharmaceuticals and personal care products (PPCPs). Compounds such as pharmaceuticals and food products are rarely completely metabolized, leading to excretion primarily through urine and subsequent concentration in wastewater (Murray and others, 2010; Salimi and others, 2017). Some organic compounds considered PPCPs include analgesics, non-steroidal anti-inflammatory drugs, antihyperlipidemics, antihyperglycemics, antimicrobials, surfactants, synthetic hormones, fragrances, insect repellents, and stimulants (table D1) (Murray and others, 2010; Salimi and others, 2017). PPCPs have a wide range of polarities and octanol-water partitioning coefficient (K_{ow}) values affecting their partitioning in the water column and in organisms, ranging from polar compounds that are highly water soluble to hydrophobic/lipophilic compounds more likely to partition into sediments and bioaccumulate in aquatic organisms. Some of the lipophilic compounds enable them to easily enter the food chain and propagate toxic effects throughout an ecosystem (Gramatica and others, 2016). A sub-class of PPCP compounds is endocrine disrupting chemicals (EDCs), which alter functions of the endocrine system and interfere with synthesis, metabolism, binding, or cellular responses to natural estrogens (Salimi and others, 2017). Many EDCs make their way into sewage collection systems from domestic and commercial activities and are not completely removed by wastewater treatment plants (WWTPs), resulting in their discharge into streams. Some of these EDCs are biogenic (for example, 17β-estradiol and estrone), others are synthetically designed to affect biological systems like pharmaceuticals (for example, 17α-ethinylestradiol and metformin) or pesticides (for example, endosulfan and atrazine), while other consumer chemicals inadvertently cause endocrine disruption (for example, alkylphenols, bisphenol A [BPA], phthalate esters,

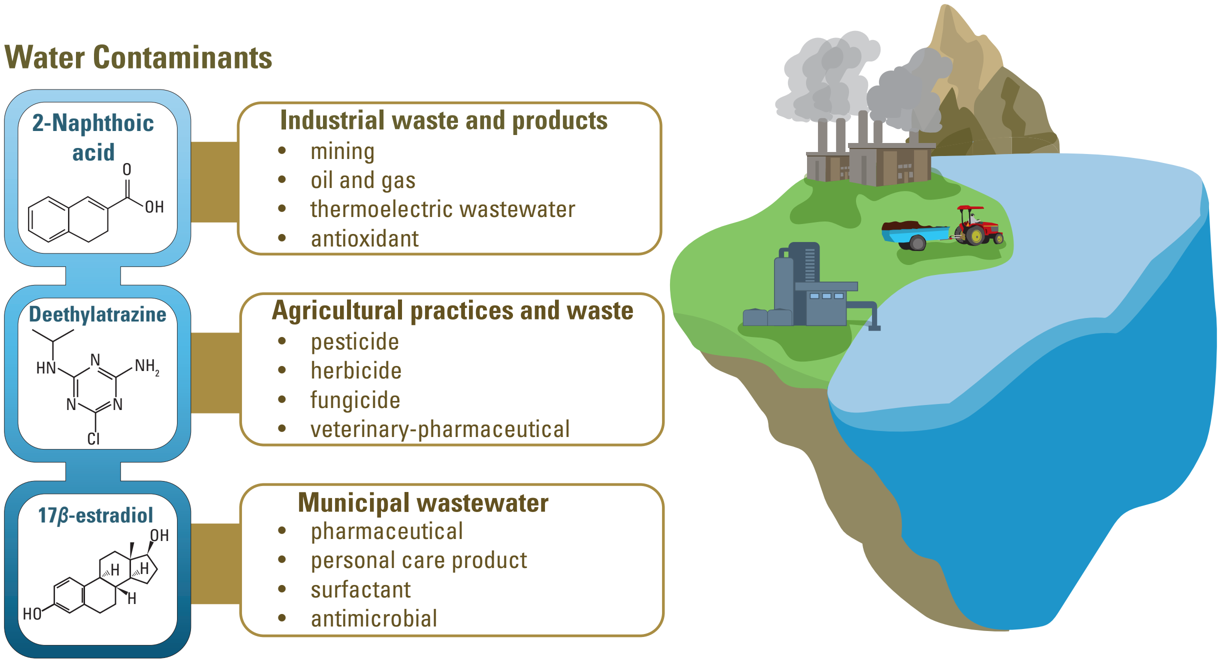

Figure D1. Diagram showing the three broad sources of contaminants of emerging concern (CECs) discussed in the text: (1) municipal wastewater, (2) industrial waste and products, and (3) agricultural practices and waste. Some key example contaminants from these sources are shown: 17 β-estradiol, 2-napthoic acid, and deethylatrazine.

Table D1. Contaminant sources and classes in relation to water use in the United States. Uses of the compound classes as well as specific examples are shown, based on Salimi and others (2017).

[NSAID, Nonsteroidal anti-inflammatory drug; PFAS, poly- and perfluoroalkyl substances; EDTA, ethylenediaminetetraacetic acid; NTA, nitrolotriacetic acid; DEET, N,N-diethyl-meta-toluamide; THMs, trihalomethanes; HANs, haloacetonitriles; HAAs, haloacetic acids; NDMAN-nitrosodimethylamine; AHTN, acetylhexamethyltetrahydronaphthalene; HHCB, hexahydrohexamethylcyclopentabenzopyran; PCBs, polychlorinated biphenyls]

Compound Class	Use	Examples
Municipal wastewater		
Analgesics	Pain reliever	Acetaminophen and acetylsalicylic acid
NSAIDs	Anti-inflammatory	Naproxen, ibuprofen, ketoprofen
Antiepileptic drugs	Treat seizure disorders	Carbamazepine and primidone
Antidepressants	Treat depression/anxiety	Fluoxetine, desvenlafaxine, venlafaxine
Antihyperglycemics	Diabetes control	Metformin, glyburide, sitagliptin
Antihyperlipidemics	Lipid regulators	Gemfibrozil, clofibric acid
Antimicrobials	Antibiotics and disinfection	Sulfamethoxazole, sulfamethazine, erythromycin, tetracycline, triclosan
Antioxidants, flame retardants, plasticizers	Plastic and resin products	Bisphenol A, bisphenol F, diethyl phthalate, tris-(2-chloroethyl) phosphate, tris-(dichloroisopropyl)phosphate
Surfactants	Detergents, water and stain resistance	Nonyphenols, octylphenols, PFAS
Chelating agents	Metal ion sequestration, water softener, solubilization	EDTA, NTA
Natural and synthetic hormones	Hormone modulation	17β-estradiol, estrone, 17α-ethinylestradiol
Insect repellant and insecticides	Pest control for fleas, ticks, roaches, white flies for pets, golf courses, turf	Fipronil, pyriprole, DEET
Herbicide	Herbicides for urban residential environments	Pendimethalin, glyphosate, dacthal
Disinfection by-products	Unwanted by-products of disinfection of drinking water and wastewater effluent	THMs, HANs, HAAs, NDMA
Other	Fragrances, stimulants, UV inhibitors	AHTN, HHCB, acetophenone, caffeine
Industrial products and waste		
Halogen-containing flame retardants	Flame retardants and aqueous film forming foam (AFFF)	Polybrominated diphenylethers, PFAS
Halogen-containing organic compounds	Heat transfer fluids and lubricants	PCBs
Antioxidants, plasticizers, flame retardants	Plastic and resin products	Bisphenol A, bisphenol F, diethyl phthalate, tris-(2-chloroethyl) phosphate, tributylphosphate
Oil and gas waste	Additives, fracking fluids, degreasers, hydrocarbons	Methyl-tertiary-butyl ether, ethylene dibromide, trichloroethane, 1,4-dioxane, polyaromatic hydrocarbons, methane
Industrial by-products	Chemical and plastics manufacturing	Dioxins, microplastics, 1,4-dioxane, PFAS
Alkylphenols	Household industrial products	Nonylphenol and octylphenol
Mining extractants	Mining and milling of natural resources	Trioctylamine, EDTA
Anti-corrosives	Aircrafts, dishwasher detergents, thermoelectric power	Benzotriazole and tolyltriazole
Agriculture practices and waste		
Carbamates	Herbicides, insecticides, fungicide	Carbendazim, benomyl and carbaryl
Chloroacetanilides	Preemergent herbicides	Metolachlor, alachlor
Chlorophenoxy acids	Herbicides	Bentazone, triclopyr
Organochlorines	Insecticides	DDT, dieldrin, endrin, endosulfan
Organophosphates	Insecticides	Diazinon, malathion, chlorpyrifos, tebupirimfos
Phenylpyrazole	Insecticide	Fipronil
Pyrethroids	Insecticides	Biphenthrin, cypermethrin
Triazines	Herbicides	Atrazine, cyanazine, simazine
Triazine	Insecticide control of aphids and white flies	Pymetrozine
Neonicotinoids	Insecticides	Imidacloprid, chlothianidin, thiacloprid, thiamethoxam
Fungicides	Fungicides	Azoxystrobin, boscalid, fluxapyroxad, metalaxyl, metconazole, myclobutanil, trifloxystrobin
Other prevalent herbicides	Herbicides	Phenylurea, isoproturon
Other prevalent insecticides	Insecticides	Propargite
Plant sterols	Phytoestrogenic effects	Daidzein, coumestrol, equol, biochanin A
Veterinary pharmaceuticals	Confined animal feeding operations	Bacitracin, arsenilic acid, erythromycin, chlortetracycline

and polychlorinated biphenyls) due to chemical structure similarities with estrogen or other natural hormones (Roy and others, 2009; Barber and others, 2012; Barber and others, 2015). Many PPCP compounds undergo biodegradation or oxidation during wastewater treatment producing TPs that are potentially more harmful than their respective parent compounds (Roberts and others, 2016; Eriksson and others, 2017). Furthermore, rising populations and water scarcity (especially in the arid southwestern United States) have led to greater proportions of treated wastewater being reused intentionally or incidentally to supplement drinking water sources and other beneficial water uses (National Research Council, 1998; Rice and others, 2013; Rice and Westerhoff, 2015; Abbott and others, 2019). Therefore, there is increasing concern for the occurrence and adverse effects of the anthropogenically introduced CECs that enter water bodies. When this water is treated as drinking water, additional concerns arise regarding the production of toxic disinfection by-products (DBPs) like trihalomethanes, haloacetonitriles, haloacetic acids, and N-nitrosodimethylamine, which are formed when disinfectants (chlorine, chloramine, ozone) react with naturally occurring organic matter (Richardson and others, 2007; Weisman and others, 2019; Weisman and others, 2021).

It also is important to understand the lesser-known water-quality effects from mining, thermoelectric power plant cooling, and aquaculture water being used and returned to the hydrologic environment via direct and indirect discharges. There are fewer studies investigating the water-quality effects of return flows coming from storm water drainage, aquaculture, and agricultural biosolids applications, which create complex chemical mixtures of pesticides, fertilizers, pharmaceuticals and PPCPs, all exposing aquatic organisms to impaired water quality, potentially at critical life stages or habitats (Australian and New Zealand Environment and Conservation Council [ANZECC] and Agriculture and Resource Management Council of Australia and New Zealand [ARMCANZ], 2000; Nowell and others, 2014; Nowell and others, 2018; Masoner and others, 2019).

Industrial Products and Waste

The production of goods and materials used in modern urban environments involves the use of a variety of chemicals that can have deleterious effects on water quality. Industrial organic chemicals used in manufacturing and production processes include antioxidants, flame retardants, surfactants, perfluorates, phenols, phthalates, triazoles and others (table D1) (Murray and others, 2010). Antioxidants toxic to aquatic organisms, such as butylated hydroxyanisole and butylated hydroxytoluene, are used in the production of rubber, petroleum products or to preserve food (Kolpin and others, 2002). Per- and polyfluoroalkyl substances are used extensively in firefighting efforts at military bases and airports (for example, perfluorooctane sulfonic acid, aka PFOS), while a multitude of other PFAS compounds, such as perfluorooctanoic acid (PFOA) and other perfluoroalkanoic acids, are widely used in consumer products for their non-stick properties, water resistance, and stain resistance (Navarro and others, 2016; Suthersan and others, 2016; Zhang and others, 2016). These compounds are increasingly important for water resource managers due to our growing understanding of toxicity effects and prevalence (Clara and others, 2009; Sunderland and others, 2019; Ankley and others, 2021; MacGillivray, 2021), as they are ubiquitously found in municipal and industrial wastewater effluents and biosolids (Zhang and others, 2016; Eriksson and others, 2017; Gallen and others, 2018), landfill leachates (Lang and others, 2017), and even agricultural sources (Kolpin and others, 2021). Phenols are commonly found in epoxy resins and plastics and some compounds, such as nonylphenol and BPA, are considered endocrine disrupters (Murray and others, 2010). Most phthalate esters tend towards hydrophobicity, but low molecular weight phthalates such as dimethyl phthalate and diethyl phthalate used as solvents in PPCPs and insecticides, and time released pharmaceuticals are more soluble, thus contributing to widespread detection of these compounds in the aquatic environment (Murray and others, 2010).

In addition to the manufacturing of materials and goods, industries at the intersection of anthropogenic activity and the natural environment, such as oil and gas production and mining, can contribute to the input of contaminants into water bodies of concern. Contaminants of concern for oil and gas exploration and production activities, including spills and waste disposal sites, are both inorganic and organic in nature. For example, in North Dakota, the number of oil and gas waste-fluid releases has been increasing from 2008–2015, often due to pipeline leaks or spills during transfer from storage tanks (Cozzarelli and others, 2021). These oil and gas wastes contain contaminants such as salinity, barium (Ba), strontium (Sr) and trace hydrocarbons, some of which were detected 2.5 years (yrs) after a spill and up to 7.2 kilometers (km) downstream (Cozzarelli and others, 2021). Similarly, downstream from an oil and gas waste facility in West Virginia, waters contain elevated specific conductivity, chloride (Cl^-), and radium (Ra) (Akob and others, 2016). Another oil and gas persistent contaminant stemming from leaking underground storage tanks is methyl tertiary butyl ether (MTBE), which was added to gasoline in the United States beginning in the mid-1980s and by the early 1990s was the second most frequently detected volatile organic compound in shallow urban groundwater (Squillace and others, 1996). Microbial degradation rates of MTBE are relatively slow compared to other gasoline components (Landmeyer and others, 1998), and thus can remain an issue at some spill sites long after its use has been discontinued.

Mining waste contamination concerns are typically focused on heavy metals, which are classified as CECs, and improvements in analytical techniques allow for detection of lower concentrations that previously went unnoticed. In the Upper Colorado River Basin, heavy metals such as lead (Pb), cadmium (Cd), zinc (Zn), arsenic (As), and copper (Cu) from mining activities threaten water quality. Silver mining in the Gunnison National Forest at the Standard Mine site, about 7 km west of the town of Crested Butte, for example, has led to heavy metal contamination of soil, ground, and surface waters (Nash, 2002). Deposition of heavy metals into nearby Elk Creek has also caused contamination of Coal Creek and other downstream water bodies (Nash, 2002). Mining contaminants are not only an issue due to the transport of these constituents to vulnerable water bodies, but also because biogeochemical conditions change along a flow path and may be different in the receiving water body. Factors such as pH, redox conditions, salinity, total suspended solids, and microbial communities vary spatially, and influence metal contaminant speciation, toxicity, and bioavailability. The effects of anthropogenic extractants and chelating agents, such as trioctylamine and ethylenediaminetetraacetic acid (EDTA), used during extraction and milling processes are largely ignored in the public literature, although their aquatic concentrations are high enough to influence shifts in geochemical speciation and bioavailability of in-stream metals. Therefore, to best assess long-term water risk management of Integrated Water Science (IWS) basins, it is essential that sources of contamination are identified, and that contaminant chemistry in receiving water bodies is understood.

Agricultural Practices and Waste

The production of agricultural products (that is, foodstuffs, cotton, hemp, turf, livestock) is another example where anthropogenic activity intersects with the natural environment and contributes CECs to the aquatic environment. Agriculture is vital for human survival but runoff and (or) waste from agricultural practices can introduce CECs, such as pesticides, veterinary pharmaceuticals, nitrification inhibitors, surfactants, and estrogenic hormones to water bodies (Kolpin and others, 2002; Murray and others, 2010; Salimi and others, 2017; Woodward and others, 2018; Woodward and others, 2019). Pesticides can be further classified as herbicides, insecticides, fungicides, rodenticides, and miticides, all of which are designed to control weeds, pests, and fungi via prevention, destruction, or repulsion to enhance food production (de Souza and others, 2020). It is estimated that 10 percent of pesticides applied to soil reaches non-target areas, an amount that is enhanced if it rains shortly after application (Schulz, 2004). Although few pesticides have been officially classified as persistent organic pollutants as of 2020, many fall into this category in that they are persistent, toxic, and demonstrate long-range environmental transport (de Souza and others, 2020).

The occurrence and synergistic biological effects of most pesticides and their TPs are not fully understood, especially in the context of responses to changes in flow conditions or timing of applications (Murray and others, 2010; Nowell and others, 2014; Nowell and others, 2018; Norman and others, 2020; Mahler and others, 2021). A fair amount of literature can be found discussing the concentrations and water-quality effects of specific pesticide chemicals (that is, insecticide, herbicide, or fungicide) as they enter the freshwater environment following irrigation or storm runoff events (Stone and others, 2014; McKnight and others, 2015; Miller and others, 2020). For example, atrazine is an herbicide that historically has been widely spread on soybean and corn crops across large areas (de Souza and others, 2020). With approximately 80 million pounds applied annually, atrazine is the most common pesticide contaminant of ground and surface water in the United States and has a half-life of a year or more (Solomon and others, 1996). It has been widely detected in Europe despite a ban in 2003 (de Souza and others, 2020). This compound is considered an endocrine disruptor, as demonstrated by demasculinization (chemical castration) and complete feminization in adult male frogs following environmental exposure (Hayes and others, 2006a, 2006b, 2010). Other triazine herbicides such as cyanazine and simazine have similar chemical structures and modes of action but have not been studied as throoughly. In general, the effects of pesticides on endocrine disruption are not well known, particularly when TPs are also considered.

Agricultural chemical inputs to water bodies can be found throughout the United States. General agricultural practices can contribute to harmful algal blooms (HABs) in the Illinois River Basin. On a broader scale, the use of pesticides across the United States has been linked to the growth of HABs (Harris and Smith, 2016; Stackpoole and others, 2021). Therefore, manufacturing, processing, storage, and use of agricultural chemicals are potential sources of contamination for organic contaminants such as pesticides in basins where agricultural land use is prevalent. Finally, spills and pesticide handling and mixing facilities should also be considered as potential sources of agricultural CECs (Haack and others, 2015).

Gap Analysis and Approaches

Gap 1. Wastewater Reuse and Anthropogenic Return Flow Relations to Water Quality

Knowledge Gaps

Key knowledge gaps involve water-quality degradation effects associated with various water use categories (table D2). The major knowledge gaps in understanding the contaminant and water-quality relationships between water use, reuse, and sustainability of high-quality water resources are:

1. Water-quality requirements and effects of the various water use categories and associated water-quality degradation effects (described later in this section).
2. The major drivers and mechanistic processes controlling exposure pathways and adverse effects to human and aquatic organism health as noted in the companion Open-File Report to this publication, their chapter C "Anthropogenic and Geogenic Contaminant Bioexposures Affecting Aquatic Ecosystems" (Harvey and others, 2024).
3. Wastewater discharge and other anthropogenic return flows with their associated chemical loads (for nutrients, geogenics, and CECs) need to be quantitatively incorporated into predictive hydrologic and solute transport models.
4. The transference from source water of intake to different receiving water of return flow.

The USGS can seek ways to better characterize what the water-quality needs are for some of the important water use categories, especially in relationship to salinity or currently

Table D2. Summary table for contaminants of emerging concern gap analysis for beneficial water use in the United States.

[CEC, contaminants of emerging concern; WWTP, wastewater treatment plant; IWS, Integrated Water Science; TP, transformation product; USGS, U.S. Geological Survey.]

Topic	Knowledge Gap	Importance	Proposed Approaches	References
Wastewater reuse and anthropogenic return flow relationship to water quality.	Determination of output degradation effects from consumptive use on water quality and CEC fate, as well as corresponding assessment of the effect of CEC input to water bodies of concern	Anthropogenic water use-and-loss effects on CEC concentrations could lead to adverse water-quality and biological effects. Water-quality needs from dominant water use categories are unclear, especially in relationship to currently unregulated CEC.	Field and laboratory-based studies of CEC fate in relation to landscape use and WWTP. Compilation of a water use requirements database to identify critical water-quality study needs.	Kolpin and others, 2002; Rice and Westerhoff, 2015; Barber and others, 2019; Weisman and others, 2019.
Legacy point sources	Identification of legacy point source sites near IWS basins and corresponding hydrogeochemical and geophysical processes and parameters affecting CEC transport and fate	Legacy point sources and corresponding flow paths to IWS basins could be introducing CECs with detrimental water-quality effects	Collaboration with local and State stakeholders to locate point sources of interests. Geochemical water-quality analysis and collaboration with geophysicists to understand systems.	Lapworth and others, 2012; Akob and others, 2016; Cozzarelli and others, 2021.
TPs of CECs	Ability to measure TP concentrations in water bodies of concern and better understand TP biogeochemistry	TPs may be more soluble, toxic, and concentrated compared to parent compounds but are currently not measured. Biogeochemical behavior is understudied.	Development of methods to better quantify TPs of interest and assess toxicity in collaboration with the USGS Ecosystems Mission Area. Assessment of sampling frequency and hydrogeological behavior.	Kolpin and others, 2004a; Barber, 2014; Bekins and others, 2016; Mahler and others, 2021.

unregulated CECs. It also would be useful to develop an assessment approach for determining gradations of water-quality requirements that can be universally applied to water use applications. A summary of known inflow water-quality suitability requirements for the nine USGS defined water use categories plus effects to aqueous ecosystem health, is provided in table A1 in chapter A of this report. Thermoelectric and mining uses typically have minimal water-quality requirements, whereas public water supply is highly regulated and maximum contaminant levels for biogenic and anthropogenic contaminants are strictly enforced. Some of the other water uses are difficult to succinctly summarize by category since many of the water-quality requirements are industry specific or process dependent, but a universally applied water-quality requirement scheme could be useful.

There is an even larger gap in our knowledge of the water-quality degradation that occurs when anthropogenically used water is returned to natural waters (Rice and Westerhoff, 2017). Consumptive use of water occurs when an anthropogenic activity draws from available water supplies within a basin and returns only a portion or none of the withdrawn water to the basin. Water might be lost to evaporation (for example, thermoelectric cooling or reservoir storage), evapotranspiration (for example, agriculture and landscaping), or incorporation into a product, such as a beverage, and shipped out of the basin (Dieter and others, 2018). Approximately 97 percent of the 133 billion gallons per day (Ggal/d) withdrawn for United States thermoelectric power in 2015 was returned to natural waters (Dieter and others, 2018). The addition of thermal energy (temperature increases), salinity (evaporative concentration), and specific contaminants, such as corrosion inhibitors and antimicrobial chemicals, to the returned water could have dramatic effects on downstream water quality and warrants further investigations. Concerns include thermal pollution of sensitive riparian ecosystems that may be located where cooling water outflows are returned to surface waters. For water uses like crop irrigation, with high consumptive use, concentration effects on the return flow can raise concerns for water-quality degradation. Of the 118 Ggal/d of groundwater and surface water and the 0.669 Ggal/d of reclaimed wastewater used for irrigation in the United States in 2015, it is estimated that 62 percent was consumed through evaporation, evapotranspiration, or incorporation into the irrigated crops (Dieter and others, 2018). The estimated 38 percent of irrigation water returned to natural waters will carry the load of agricultural chemicals used, flush geogenic constituents from the soils, and have concentration effects, all leading to potentially unacceptable levels of salinity, toxic metals, or anthropogenic contaminants with adverse biological effects.

Approaches to Fill Knowledge Gaps

To assess the effects of intentional or incidental wastewater and return-flow water reuse, and address the gaps discussed above, the following approaches are suggested. A systematic review of the nine water use categories is suggested to prioritize those uses with the greatest potential for causing water-quality degradation in critical water resources. This review also will identify the water return flow categories most suitable for reuse, along with barriers that hinder the incorporation of planned, purposeful water reuse into a community's water planning portfolio (U.S. Environmental Protection Agency [EPA], 2020). One framework for evaluating water reuse science is the National Water Reuse Action Plan (EPA, 2020), which provides useful data and lessons learned to advance the consideration of purposeful water reuse to improve the security, sustainability, and resilience of our Nation's water resources in the face of a changing climate. It would be useful to expand this framework to develop an assessment approach for determining gradations of water-quality effects of return flows based on type and compare those with established toxicity or water-quality benchmarks in combination with a universally applied water-quality requirement framework for each of the beneficial use categories.

Table D1 summarizes the well-known contamination sources and classes in relation to water use. Reviews of relevant documents and databases could be developed to prioritize lists of CECs to consider in IWS basins' investigations (Kolpin and others, 2002; Buxton and Kolpin, 2005; Nowell and others, 2014; Bradley and others, 2016, 2017; Hladik and others, 2016; Conley and others, 2017a, 2017b; EPA, 2021a, b). This work aims to provide evaluations of water-quality assessments that could be improved or need more studies to better understand the occurrence, fate, and biological effects of CECs.

In compiling water-quality effects of the nine USGS defined water uses plus ecosystem health, we could develop a scheme that allows for cross comparison of the different water-quality or toxicity benchmark measurements used in different aspects of water assessment, such as maximum contaminant levels (MCLs) for drinking water versus aquatic life benchmarks used for aquatic organism health. The table of compiled water-quality benchmark values should be annotated with the: (1) definition of the benchmark concentration unit and description of what it means to have this benchmark value exceeded, (2) source type of the data, measured or predicted (for example, computational and modeled simulations), with citations, and (3) quality of the data with information on limitations, uncertainties, and underlying assumptions. This qualitative information will be important to data users when interpreting water quality data and trying to make water management decisions. The importance of knowing what is meant when exceedances are observed can be illustrated with the example of Canadian water-quality guidelines, which are intended to protect all forms of aquatic life during all stages of the aquatic life cycle and should not be exceeded at any time (https://ccme.ca/en/current-activities/canadian-environmental-quality-guidelines); in contrast, EPA's criterion continuous concentration (CCC) is a chronic exposure benchmark that applies to four-day average concentrations, and is intended to protect 95 percent of aquatic species, and should not be exceeded more than once in three years. Moreover, important water management decisions should be made with a clear understanding of the quality of the data. For example, a sediment benchmark for aquatic life might be: (1) measured based on spiked sediment bioassays, (2) predicted from a measured toxicity value in water using the soil organic carbon partitioning coefficient (K_{oc}) and equilibrium partitioning theory, or (3) predicted based on K_{ow} only. The quality of the benchmark in these cases would decrease from (1) to (3).

Municipal wastewater is a prime example of a complex chemical mixture of CECs that is often reused and the point source discharge of WWTPs allows for direct correlation between chemical loads and resulting stream concentrations. For these reasons, we suggest initially focusing on municipal and industrial WWTPs in future IWS basins for field and laboratory-based studies to address the interactive effects of complex mixtures of CECs and their TPs on water quality, similar to work done by USGS colleagues in Muddy Creek, Iowa (Zhi and others, 2020, 2021; Webb and others, 2021). Initial landscape assessments could be conducted to identify additional CEC sources, in addition to WWTPs, and would entail collaborations with local stakeholders. Subsequent investigations could be done to fill in other data gaps from other return flows from surrounding landscape uses (for example, agricultural) and anthropogenic activities (for example, thermoelectric). Measurements of specific CECs would depend on IWS basin needs and require state-of-the-science measurements using gas chromatography-tandem mass spectrometry (GC-MS/MS) and liquid chromatography-tandem mass spectrometry (LC-MS/MS) techniques for organic contaminants and inductively coupled plasma-mass spectrometry (ICP-MS) and optical emission spectroscopy (ICP-OES) for toxic metals and trace element contaminants. In addition to targeted and unknown compound measurements, a combination of geochemical (for example, conductivity, pH, dissolved oxygen, nutrient concentrations) and hydrologic (for example, streamflow and flow velocity) measurements could be used to assess CEC sources, fate, and transport. These field measurements also would involve assessing water quality of surrounding natural waters in relation to WWTPs and other sources to determine the effects of reuse on water quality and aquatic organisms or risks to drinking water sources, building upon previous investigations of complex mixtures like those undertaken in Boulder Creek, Colorado, and Fourmile Creek, Iowa (Bradley and others, 2007; Barber and others, 2011; Barber and others, 2013; Zhi and others, 2020; Zhi and others, 2021). Once specific CECs in IWS basins are identified through field investigations, laboratory-based studies could be carried out to establish transformation rates, TPs, and potential health risks needed as input parameters for wastewater and hydrologic transport modeling of the complex mixtures.

Most of the organic and inorganic CECs cannot be monitored continuously, but instead require discrete sampling. As with the point-source legacy contaminants, the analyses require complex, labor-intensive, and relatively expensive (for example, GC-MS/MS and LC-MS/MS) techniques for organic contaminants. WMA could promote research-based development of new analyses and remote sensing techniques for CEC assessments around the nation that could support stakeholder-driven decisions. The USGS Actionable and Strategic Integrated Science and Technology (ASSIST) projects in the Colorado River Basin are examples of interdisciplinary science and application of advanced techniques for complex stakeholder driven challenges. For example, recent proof-of-concept studies in the Colorado River Basin during 2022–2023 have tested and begun environmental validation procedures for the following advanced techniques: (1) novel Turner C6P fluorescence sensors with continuous remote readings of fluorescence measurements that can characterize organic water-quality constituents (including screening for risk of wastewater-driven CEC contamination), (2) in-stream solid-phase extraction samplers (“SPE-bots”) allowing enrichment of trace organic contaminants (that is, PFAS, PPCPs, EDCs, pesticides) for simplified sample processing and analysis in the lab, and (3) molecularly imprinted polymer-modified electrochemical sensors (MIPMECS) as an innovative technique for in-stream measurements of PFAS contaminants. Another approach is development and modification of analytical methods (likely mass-spectrometry techniques) to provide a rapid screening method for detecting priority CECs and proxies for hazardous aqueous chemicals coming from different sources, different chemical classes, and with different modes of action. This method would focus on limiting the total constituents analyzed and using important proxy chemicals to represent chemical classes and (or) source categories, along with incorporation of automated sampling and processing steps to reduce analytical costs and improve data delivery times, both of which can be limitations of existing CEC measurement techniques. These screening methods for CECs and relevant proxy constituents would provide essential and timely measurement data for calibration and ground-truthing of CEC hydrologic transport models. It would also help to identify water resources highly affected by CECs that warrant additional monitoring with more comprehensive water-quality analyses.

Gap 2. Legacy Point Source Sites of Contaminants of Emerging Concern

Knowledge Gaps

CECs in surface water and groundwater may migrate from a point source to a water body of interest. Point-source pollution originates from discrete locations and inputs into aquatic systems can be defined in a spatially discrete manner (Lapworth and others, 2012). Some point sources are the result of accidents such as oil or waste spills, while others may be the result of decades-long (legacy) anthropogenic activity such as landfills or WWTP effluent discharges. Many legacy landfills were constructed with little or no leachate controls systems, posing unquantified threats to local water bodies (Hepburn and others, 2019; Masoner and others, 2019). The scale of this threat depends on a variety of factors including leachate composition, distance from water bodies, and local geochemistry and geology (Masoner and others, 2014, 2016; Stamps and others, 2016; Talalaj and Biedka, 2016; Hepburn and others, 2019). Just as varied as the types of point sources are the types of contaminants that stem from them, ranging from metals such as Pb, Zn, and Cd, to organic chemicals such as volatile organic compounds (VOCs,) polychlorinated biphenyls (PCBs), light non-aqueous phase liquids (LNAPLs), 1,1,1-trichloroethane (TCA), trichloroethylene (TCE), creosote, phthalate esters, and a wide range of PPCPs (table D1). Geochemical parameters including salinity, pH, dissolved oxygen, and dissolved organic carbon as well as sediments have a distinct influence on the fate of legacy CECs in surrounding water bodies (Hepburn and others, 2019). These factors effect CEC degradation, transformation, transport, and bioavailability in receiving water bodies adjacent to a legacy point source. Furthermore, complex geological and geophysical characteristics, such as low-permeability sediments, may allow legacy point source sites to act as long-term sources of CECs (de Lambert and others, 2021).

The WMA initially identified three IWS basins for intensive study: (1) the Delaware River Basin, (2) the Illinois River Basin, and (3) the Upper Colorado River Basin. These basins are being monitored to understand distinct processes such as the effects of drought on water supply in the Delaware River Basin, cold-region snow and ice processes in the Upper Colorado River Basin, and nutrient contributions to HABs in the Illinois River Basin. Legacy point-source contamination has links to all these processes. For example, after a drought there will be less water available for diluting contaminant input from a point source (Kolpin and others, 2004b). In cold regions, snow and ice melt during spring may cause a surge of contaminant flow from mining waste during spring runoff. Finally, HABs are influenced by pesticides, as described above in the status of knowledge. Therefore, as intensive studies of the basins continue, it is important to consider the effect of legacy point-source contamination and associated CEC’s on water-quality processes to understand overall water body and ecosystem health.

Though there are many potential legacy point-source sites surrounding IWS basins and we discuss a few examples, this is by no means an exhaustive discussion. For example, there is a site of concern stemming from oil spills in Bridgeport, New Jersey, 2 miles south of the Delaware River (Hochreiter and Kozinski, 1985; Kozinski and others, 1990). This site housed oil waste from 1960–1981 and caused widespread damage to surrounding wetlands as early as the 1970s. The groundwater is contaminated with VOCs, PCBs, and LNAPLs and the underlying aquifer is a source of drinking water (Hochreiter and Kozinski, 1985; Kozinski and others, 1990). Another site within the Delaware River Basin is the Cinnaminson Township, New Jersey, where groundwater is contaminated with a suite of organic contaminants including TCE, benzene, cis-1-2, dichloroethane and vinyl chloride. Overall, oil refinery effluents and crude oil spills have affected the Delaware River and the Delaware Bay, though studies are currently limited (Hall and Burton, 2005; Habicht and others, 2015; Walker and others, 2016).

Many legacy point-source sites that may be affecting IWS basins involve contaminated groundwater from spills and improper disposal of commonly used solvents such as TCA and TCE, along with stabilizer chemicals such as 1,4-dioxane. Long-term exposure to 1,4-dioxane causes kidney and liver damage; acute exposure can result in death (Pollitt and others, 2019). Remediation efforts for TCA and TCE over the past 40 years were not designed to remove the very soluble 1,4-dioxane from contaminated groundwater sites, leaving a continued legacy CEC (Adamson and others, 2014). For example, in a study of greater than 2,000 California groundwater sites affected by chlorinated solvents, 76 percent had co-occurrence of 1,4-dioxane with TCA, many with 1,4-dioxane concentrations three orders of magnitude above the 0.67 micrograms per liter (µg/L) EPA drinking water standard (Adamson and others, 2014). Use of 1,4-dioxane as a solvent in consumer products is not regulated. Because 1,4-dioxane is recalcitrant to conventional wastewater and drinking water treatments there are significant numbers of drinking water sources potentially exposed as the result of wastewater discharges (Adamson and others, 2017; McElroy and others, 2019). Thus, 1,4-dioxane is an example of a legacy and current use CEC with substantial data gaps on occurrence, fate, and biological effects.

While the sites described here offer key examples of legacy point source contamination, it also is vital to consider lesser-known legacy point sources of CECs that are unique to the water body of interest. CECs at local point source sites will depend on a breadth of anthropogenic activities and proximity to urban areas (that is, manufacturing sites and landfills). Working with local stakeholders to identify these sources is an essential step toward tracking and predicting CEC fate.

Approaches to Fill Knowledge Gaps

To characterize the effects of legacy point source pollution, sites can first be identified in the IWS basins. Some potential legacy point source sites include municipal and industrial wastewater discharges, landfills, chemical spills, food processing plants, pharmaceutical manufacturing plants, and so forth; however, this is not a complete inventory. It is unclear exactly how many legacy point-source sites exist in these areas, with potentially poorly characterized sites that are contributing to surface and (or) groundwater contamination. Searches of national databases and collaborative efforts between the USGS and State and local agencies can help identify legacy point-source sites and assess the degree of water-quality impairment at these sites and the associated threat they may pose to IWS basins. Once identified, sites could be ranked based on threat to the basin in terms of CEC concentrations, toxicity, reactivity, and transformation potential.

Water-quality parameters at major legacy point-source sites of interest could be measured using data loggers, discrete samples, in-situ passive and continuous samplers, and other water-quality monitoring tools available to the USGS. Together, available discrete sample data and continuous information about pH, salinity, dissolved oxygen, and temperature would provide a record of baseline geochemical conditions over time. With regards to CECs, there is an overarching lack of data and understanding as it relates to the sources, fate, and effects of these constituents. Initial characterization of aqueous geochemical parameters and CEC concentrations in relation to a known legacy point-source site would allow for relationships between these parameters and CEC fate to be established. Geochemical, surface-water, and groundwater modeling could then be leveraged with in-situ measurements to enhance predictive capabilities of CEC fate. However, it must be noted that CEC geochemical behavior is extremely complex and while this work could potentially improve predictions, it is not expected to be a one-size-fits-all understanding of CEC geochemistry.

In addition to measuring water quality at point-source sites, long-term measurements along groundwater and surface-water flow paths to water bodies within IWS basins could also be analyzed to better understand the role of water quality and aqueous geochemistry in contaminant fate and transport from legacy point source sites. Collaboration with geophysicists would allow for the use of electromagnetic and thermal imaging techniques that can be used to track the fate of plumes (Ball and others, 2020; Briggs and others, 2020). These data, along with physicochemical properties of the chemicals that control fate and transport, could be incorporated into hydrologic transport models that could be used to understand groundwater and surface water interactions in relation to points of discharge. These models could help to predict CEC behavior from point sources in current and future IWS basins and potentially help to assess risk to downstream aquatic organisms and (or) drinking water sources.

Direct measurements of contaminant concentrations (for example, gas chromatography with mass spectrometry [GC-MS], liquid chromatography with mass spectrometry [LC-MS], ICP-MS, and ion chromatography) and biological assessments (for example, field and lab bio-exposure experiments, tissue analysis of native aquatic species, cellular assays, genomic and transcriptomic technologies) from legacy point source sites and along flow paths in IWS basins will be an important aspect in assessing their effect. Many organic and inorganic CECs require discrete sampling and complicated analyses due to low concentrations and complex mixtures. The chemical structures of many CECs are not conducive to typical real-time monitoring equipment (for example, potentiometric, spectrophotometric, or fluorometric analyzers). By focusing initially on the primary processes of interest at each IWS basin (drought conditions in the Delaware River Basin, HABs in the Illinois River Basin, and snowmelt-driven processes in the Upper Colorado River Basin), CECs that affect each of these processes can be targeted. For example, in the Illinois River Basin, fertilizers and pesticides from legacy point sources such as chemical storage and (or) spills can be measured along flow paths and changes in concentration noted to discern their potential influence on HABs growth. Conversely, in the Upper Colorado River Basin, which is influenced by mining waste, it is logical to focus on metals and metalloids whose mobilization and aqueous concentrations will be affected by snow and ice melts on a seasonal basis. These are just a few examples of potential target contaminants, allowing for room and flexibility to expand in new directions.

Gap 3. Transformation Products as Contaminants of Emerging Concern

Knowledge Gaps

Organic contaminant studies have focused primarily on the original compounds (that is, parent compounds) released into the environment. However, it has been recognized for decades that TPs of pesticides and consumer product chemicals may be more prevalent than the parent compounds in groundwater (Field and others, 1992a; Field and others, 1992b; Kolpin and others, 2000, 2004a; Bexfield and others, 2021; Fisher and others, 2021). Moreover, because occurrence of TPs is common in groundwater, baseflow is an important source of TPs to streams (Squillace and others, 1993). Notably, some TPs are more toxic than their parent compounds, as is the case for polyaromatic hydrocarbons (PAHs) (Knecht and others, 2013). For some compounds, such as triclosan, the TP methyl triclosan can be the predominant form found in surface water (Lindström and others, 2002). In a nationwide survey of contaminant mixtures in streams (Bradley and others, 2017), the most frequently detected compound was an insecticide TP (desulfinyl fipronil). In another national study, the TP desulfinyl fipronil was detected in over 90 percent of stormwater samples (Masoner and others, 2019). Thus, TPs of hydrocarbons (Bekins and others, 2016), pesticides (Mahler and others, 2021), and wastewater compounds (Barber, 2014) are ubiquitous in water, but their formation, persistence, and toxicity are poorly characterized. Gaining a better understanding of TPs is important for water assessments because overall toxicity of contaminants in water could be vastly underestimated if TPs are not also considered.

Recent examples in the literature illustrate how TPs are affecting United States water quality. For example, a TP of a tire antioxidant has been linked to Coho salmon (*Oncorhynchus kisutch*) mortality in the Pacific Northwest (Tian and others, 2021). The TPs of the insecticide fipronil are more stable than the parent compound and show ecological effects at much lower values than the EPA fipronil chronic invertebrate benchmarks (Miller and others, 2020). A major issue with TPs is that there are few health-based screening criteria. TPs may be more prevalent and present in higher concentrations than the parent compounds (Kolpin and others, 2000). In some cases, they are more soluble and polar than parent compounds and thus more mobile and persistent. Furthermore, they may be undetected because of a lack of standard methods (Mahler and others, 2021). Recognition of TP prevalence is growing as new methods are developed to identification and quantifications. USGS can now measure more than 100 pesticide TPs (Mahler and others, 2021). Recent results show that the frequency of sampling is very important for evaluating whether stream concentrations exceed aquatic benchmarks (Norman and others, 2020). Sampling strategy is also important, as hydrologic-based sampling provides a better picture of pesticide concentrations in streams (Hladik and others, 2014).

Approaches to Fill Knowledge Gaps

A key approach needed for this work is to determine a sampling frequency strategy for transformation products of pesticides. It has been established that daily sampling reveals exceedances that are not apparent in weekly samples (Norman and others, 2020). Because daily samples may be impractical, research is needed to determine alternate approaches. Previously, sampling strategies based on hydrologic events have been successful (Hladik and others, 2014; Woodward and others, 2018; Hama and others, 2021). Future strategies may involve a combination of hydrologic event-based approaches, passive sampling devices, autosamplers or proxy methods.

More research on TP toxicity will facilitate development of meaningful screening criteria. Of the 116 pesticide transformation products measured by Mahler and others (2020), only one-quarter have an aquatic life benchmark. Often the toxicity of the parent compound is substituted for the TP, but this may be too high or low. Furthermore, the existing benchmarks may be for less sensitive species than are affected in the streams. In the case of petroleum hydrocarbons and PPCPs, very few toxicity benchmarks of parent compounds or TPs exist. Addressing this gap may involve working with toxicologists in the USGS Ecosystems Mission Area and other Federal, State, and local agencies.

In many cases, the reporting levels for TPs are higher than those for the parent compounds, leading to fewer detections. New methods that include more parent compound and TP pairs also are needed, as many potentially important compounds are not measured. Often the problem is a lack of available standards. Continued methods development on quantifying additional TPs and lowering existing reporting levels could be carried out by the USGS's National Water Quality Laboratory, the Organic Geochemistry Research Laboratory in Kansas, the Organic Chemistry Research Laboratory in Sacramento, and other USGS laboratories (https://www.usgs.gov/science/laboratories).

Often TPs are formed in groundwater and subsequently discharge to surface water (Squillace and others, 1993). Thus, TPs of pesticides are most concentrated in streams during baseflow (Mahler and others, 2021). In some cases, TPs of pesticides banned for a decade are still present in surface water suggesting long transit times in groundwater (McKnight and others, 2015; Mahler and others, 2021). Predicting the impact of TPs on water quality may require research relating to fossil fuel, pesticide, and PPCP use, parent compound and TP formation rates, transit times in groundwater, and rate of discharge to surface water. Improved methods for quantifying TP transport and transit times in groundwater is a cross-cutting issue affecting many contaminants including CECs, nutrients, geogenics, and salinity.

Concerns about the health effects of contaminant mixtures together with the impracticality of quantifying thousands of unregulated chemicals are motivating new toxicologic approaches. The goal of these new approaches is to discover which chemicals are of greatest concern (Diamond and Burton, 2021). Scientists in the USGS Ecosystems Mission Area (https://www.usgs.gov/mission-areas/ecosystems) use exposure-effects-driven tools. These tools assess the biological effects of a mixture or an extracted portion of a mixture. If adverse effects are observed, then chemical analyses are used to identify which chemical(s) in the mixture are responsible. Collaborations among WMA and Ecosystems Mission Area scientists can foster use of these new toxicological approaches.

Expected Outcomes

The wide variety of CECs, their complex interactions, and the ever-expanding list of compounds make understanding their fate and prioritizing research an extremely challenging task. This document does not address every knowledge gap that exists with respect to CECs, nor does it offer what should be considered sole approaches. Instead, we propose to address some of the most pressing gaps in knowledge as they relate to current WMA priorities. The complexity of understanding and predicting the fate, geochemical drivers, water-quality effects, and biological effects associated with CECs can be addressed by interdisciplinary teams and inter-mission area and interagency collaborations. Below are some key outcomes anticipated from this work.

- Provide novel results necessary for improved modeling capabilities, create much needed databases, and begin to address the many gaps in literature related to CEC fate, sources, and effects.

- Assess water-quality requirements for the dominant water-use categories in relation to currently unregulated CECs. Update open-platform databases that can be used for improved modeling inputs.

- Compile a comparative assessment of water-quality effects of the nine water use categories using science-based toxicity and water-quality benchmarks, resulting in the identification of water management changes most influential for preserving water quality and advancing sustainable use of critical water resources. This could provide valuable information for modeling that can be used in predicting water quality.

- Compile comparative assessment criteria to identify the water return flow categories most suitable for reuse in a watershed or region, along with identification of local and national barriers that could hinder the incorporation of planned, purposeful water reuse into a community's water portfolio (National Research Council, 1998; Rice and others, 2013; Rice and Westerhoff, 2015; Abbott and others, 2019). The collected data could advance the consideration of purposeful water reuse to improve the security, sustainability, and resilience of our Nation's water resources in coordination with the EPA's National Water Reuse Action Plan online platform at https://www.epa.gov/waterreuse/national-water-reuse-action-plan-online-platform (EPA, 2020).

- Identify principal legacy point-source sites and the corresponding CECs that pose some of the greatest threats to water quality and ecosystem health, specifically in IWS basins, which could further work in these basins and provide valuable information to local (State, county, city, and so forth) stakeholders.

- Characterize groundwater contaminant plumes from point-source sites in IWS basins and promote understanding of the hydrological and biogeochemical processes that contribute to plume mobilization. These data can be used to improve inputs in a variety of water-quality models and improve local stakeholder understanding of contaminant plumes needed for decision making.

- Expand, develop, and improve methods for foundational scientific activities through laboratory and field experiments for sample collection and detection of priority CECs, their TPs, and relevant proxy chemical indicators, which includes understanding the best sampling times and frequency related to hydrological parameters of a water body of concern.

- Improve toxicity benchmarks for a variety of unregulated CECs and TPs that should lead to improved predictions of water quality and suitability for different water use categories.

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