Storyline: Toxic-free water resources for healthy people and ecosystems under global change

Clean water resources are key for healthy people, the ecosystem and for sustainable economies. The ever-increasing **number and amount of chemicals** produced, used and **emitted to the water cycle** as **complex mixtures** together with unsustainable land and water use put these water resources under threat of chemical pollution together with other threats such as anthropogenic particles (see plastics storyline, Jahnke et al.), eutrophication and hydrodynamic or structural changes. The chemical pollution threat is enhanced by **climate change** resulting in a higher frequency of **flood and drought events**. Flood events are expected to mobilize chemicals stored in sediments, from urban and industrial areas and agricultural landscapes [1]. Water scarcity in drought periods reduces the dilution of discharges and can lead to **concentrations of pollutants above safe levels**. To combat water scarcity, the EU aims to implement a **circular economy for water** with adaptive measures through its circular economy action plan and water re-use regulation. **Water re-use** for agriculture and drinking water production and **novel blue-green infrastructures** to retain water in cities and landscapes will lead to **new local water cycles** in which some pollutants may successively accumulate. This accumulation **increases the risk of human and environmental exposure** to these chemicals and hence **monitoring, evaluation, maintenance and restoration of water quality is essential** to preserve human health and the water-dependent environment (Figure 1).

Our mission: With next-generation water quality monitoring and control for transforming water landscapes and novel blue-green infrastructures we enable a sustainable circular economy for toxic-free water resources that are safe for ecosystems and human use even under challenging climatic conditions. To this end, we combine smart integrated monitoring, modelling and AI-based assessment strategies with solutions for existing and future mixtures of pollutants in urban and agricultural landscapes under change. With advanced chemical analytical tools, effect-based novel assessment methods (NAMs *in vivo, in vitro, in silico*) and models we provide early pollution warnings for the environment and identify chemicals with the potential to jeopardise healthy water resources even before they reach the environment.

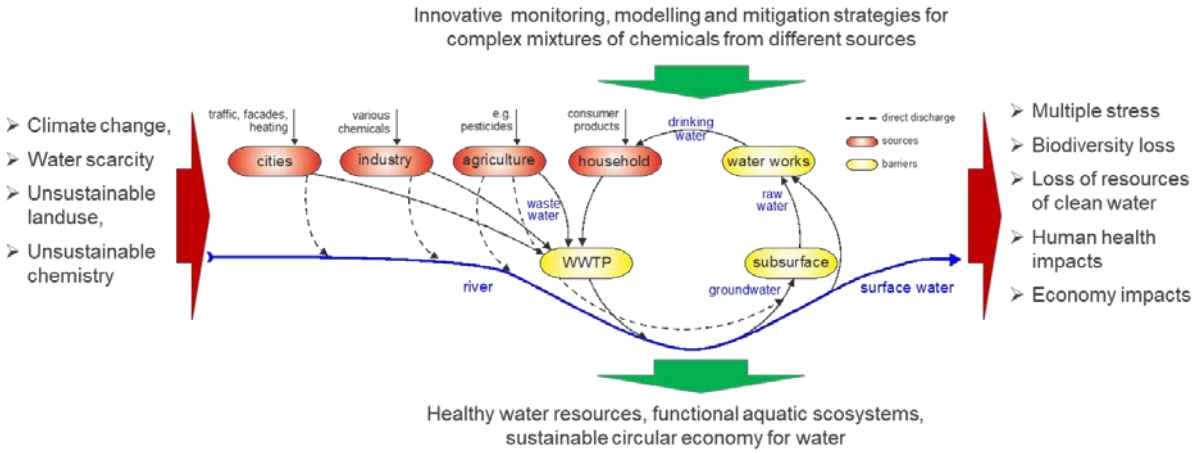

Figure 1: Turning polluted and multiply stressed water cycles to healthy water resources

Unique selling points: The combination of state-of-the-art methods in the fields of chemical screening and corresponding automated workflows, of innovative NAMs for specific under-researched effects such as neurotoxicity, of machine learning approaches to deal with chemical and toxicological complexity, of understanding of and modelling water cycles and technical mitigation methods and the

close link to the development of adaptive water management enables UFZ as a forefront runner for safe blue-green infrastructures and water landscapes under global change.

Key components of the strategy **have been developed and demonstrated** in large-scale monitoring and assessment studies, technical and non-technical measures to reduce water pollution to safe levels. **As a next step, this strategy will help to establish sustainable water cycles and blue-green infrastructures** in climate-change adapted quarters in the city of Leipzig (storyline Müller et al.) and support transformation towards resilient water landscapes (storyline Weitere et al.).

#1 Major scientific achievements

Unique monitoring toolbox to address the complexity of pollution. To assess this risk related to complex mixtures of hundreds of chemicals from multiple sources we combine innovative sampling approaches [2], with wide-scope target- and non-target chemical and bioanalytical screening [3]. We develop specialised analytical methods for pollutants that are particularly critical for the water cycle such as persistent, mobile and toxic chemicals (PMT) [4], tire wear and plastic additives [5], see also "plastics storyline", agrochemicals [6] and perfluorinated chemicals [6]. High-throughput and high-content new assessment methods (NAMs) based on effect profiling in model organisms, cellular systems [7, 8] and community assays [9] together with artificial intelligence tools [10] support the bioanalytical assessments.

Understanding the impact of pollution under global change. The impacts of urban and agricultural contaminants have been disentangled in a multiply stressed river [11]. Furthermore, we showed in microcosm studies that warming lowered critical thresholds for multiple-stressor induced shifts between aquatic primary producers [12] and depended on the exposure pathway [13]. Using UV and pesticide exposure as examples, we demonstrated that time between sequential exposures to multiple stress may have a severe impact on joint action.

Combining monitoring, modelling and impact understanding in local, national and European monitoring studies of agricultural, domestic and industrial wastewater as well as urban runoff we demonstrated the severe impacts of these sources on water quality and the key role of heavy rain events for toxic chemical mobilization. This is explained in detail below.

Solutions for pollutants in agricultural landscapes. In a national study we found that pesticide concentrations in small streams at rain events in many cases clearly exceeded regulatory acceptable concentrations [14] and exhibited neurotoxic effects [15] with severe consequences for aquatic ecosystems [14]. Using mice as a model for human health we could show that pesticides such as glyphosate can affect the allergic immune response across generations [16]. We showed that exposure and risks via the water cycle can be mitigated to acceptable levels by sufficiently wide vegetated buffer strips requiring about 4% of the agricultural land [17].

Solutions for pollutants in wastewater. Severe exceedances of risk thresholds have also been found for the vast majority of wastewater treatment plant effluents with pesticides, biocides, some pharmaceuticals [3] and endocrine disruptors [18] as major risk drivers. Based on these findings a reference mixture was established [19]. Europe-wide modelling demonstrated that the application of advanced treatment is able to reduce toxic loads to a large degree [20]. However, some persistent transformation products and many PM(T) substances still reached the water cycle [5, 21]. Using phosphorous and ammonium nitrogen as proxies we could also show the importance of spatial optimization of effluent entry points to enhance dilution capacities [22] and developed an analytical framework for determining the ecological risks of wastewater discharges in river networks under climate change [23].

Solutions for pollutants in water cycles. A better understanding of current and future water cycles and retention times under climate change-related hydrological extremes and adaptive measures is key to safeguard toxic-free water resources. Thus, we developed tools for the analysis of hydrological and (bio)chemical processes and pathways for understanding timescales and legacies of pollution, transport and degradation based on isotope analysis [26, 27]. Innovative technological approaches are being implemented to remove and chemically degrade particularly problematic chemicals such as PFAS from the water cycle [24, 25].

#2 Demonstrable networks and collaborations

(i) NORMAN: Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances; > 100 institutions from science, regulation, industry. Science-policy interface and exchange platform with the EC. UFZ: Steering committee, WG leader and project lead.

(ii) PARC: EU-funded partnership > 160 partners from science and decision making, providing new approaches for risk assessment of chemicals. Project lead on innovative monitoring tools for wastewater, contribution to NAM development, data integration, innovation in regulatory risk assessment based on multiple case studies.

(iii) eLTER: Integrated European Long-Term Ecosystem, critical zone and socio-ecological Research. Integration of chemicals into long-term monitoring.

(iv) Collaboration with BfG, UBA and GU Frankfurt. Establishment of a persistent partnership for chemical monitoring. Milestones: UFZ as Advisory Board Members of UBA-financed projects at BFG with national relevance: “Online-Portal Non-Target Screening für die Umweltüberwachung der Zukunft”, "… Reduzierung des Beitrags industrieller Abwässer an der Gewässerbelastung … (AiM)", „…prioritisation of pollutants and their sources..”

(v) IAEA. Cooperated Research Projects (F33029 and F21007) within the International Atomic Energy Agency: Understanding the importance of hydrological extremes and pollution vulnerability assessment of shallow aquifers.

(vi) Establishment of a well-working network with major water providers including Berlin, Hamburg, Dresden, Leipzig, Ruhrverband. Intensive collaboration on pollution sources.

#3 Demonstrable impact

- KGM as pilot study for the implementation of the National Action Plan Plant Protection in Germany based EU Framework Directive on sustainable use of pesticides
- WWTP studies and modelling of the impact of advanced effluent treatment on a European scale under the lead of JRC as input to the development of the proposal of a EU Directive concerning urban wastewater treatment
- Integrated monitoring as basis for remediation decisions in consideration of major stakeholders (LBGA Brandenburg, Trottheide e.V.).

#4 Demonstrable outreach products

- Model LanduseInformer estimation of in rivers of agricultural land use options. https://www.systemecology.de/landuse-informer-aquatic/index.en.html#background
- MassBank Europe (High Quality Mass Spectral Database) hosted by UFZ
- Low-cost autonomous Automatic Water Sampler (UFZ TransMarket) for high-frequency monitoring of different hydrological compartments and subsequent chemical analysis
- European PMT regulation: European Commission (2022) Delegated Regulation of 19.12.2022 amending Regulation (EC) No 1272/2008 as regards hazard classes and criteria for the classification, labelling and packaging of substances and mixtures. Collaboration with UBA.
- EU-Patent Publication of EP3873659A1 (8th Sept. 2021) „Verfahren zur Entfernung von polyfluorierten organischen Verbindungen aus Wasser mittels eines Adsorbens und dessen Regenerierung“

- TransBig-Projekt “ZeoPFAS - On-site regenerable zeolite adsorbers for the removal PFAS from wastewater“
- Licence of the product “Trap-Ox“ and the knowledge package to Intrapore GmbH who now commercially uses it
- PFAS Innovationsforum 17th Jan. 2024 together with DECHEMA addressing science, municipalities and the general public. Generating awareness on challenges and solutions.

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