Effects of global change on the emission, fate, effects and risks of chemicals in aquatic ecosystems

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Deliverable 4.3 (D23): Exposure modelling framework for estimating effects of environmental change on chemical exposure in river basins and drinking waters

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Introduction:

Climate change is expected to have large and varying impacts across Europe in the 21st Century (e.g., IPCC, 2021;EEA, 2017), including projected warmer temperatures, especially in winter in northern Europe and in summer in southern Europe. Furthermore, more frequent and intense heat waves and drought events, especially in the Mediterranean region, are expected along with more intense precipitation events, particularly in eastern Europe (e.g., EEA, 2017). These climatic changes will be happening with the backdrop of other large-scale global changes. Increased urbanization will result in more populations living in cities (EUROSTAT, 2021), agricultural practices will likely shift in response to changing environmental conditions (e.g., Nikolaou et al., 2020) and to meet rising demand (e.g., Bruinsma, 2009), and governments are likely to implement policies shifting towards a circular economy (e.g., EC, 2020). These global changes are likely to have impacts on the emissions, persistence and transformation, and fate and transport of chemicals in urban and agricultural environments, all of which will ultimately impact exposure of humans and other species to these anthropogenic chemicals.

At the time of submission of this deliverable, the ECORISK exposure work package (WP4) and an invited expert in the field (Professor Antonio Di Guardo, University of Insubria) are developing a journal article titled "Enabling prospective assessment of environmental exposure to chemicals in European agriculture under global change" (Hader and Lane et al., in prep.). The goal of this article is to develop forecasts of expected holistic changes in exposure to agricultural chemicals in Europe, as well as identify key research needs that will enable assessment of exposure and risk from these chemicals considering a range of global change drivers. The literature findings and planned modelling approach outlined in this deliverable are largely derived from the findings of this paper.

Summary of expected impacts of global change on chemical emissions, persistence, and fate & transport

Emissions of chemicals are likely to be changed by global change drivers. In response to changing pest pressures from climate change impacts, the use of pesticides is likely to increase, as well as possibly due to increased tolerance of pests to pesticides (e.g., Delcour et al., 2015). Changes in demographics are expected to drive changes in amounts of chemicals (e.g., pharmaceuticals) used in the coming decades, and will likely impact the down-the-drain emissions, thus impacting the types and amounts of chemicals that reach wastewater treatment plants and their effluent (e.g., Sjerps et al., 2017; Van Der Aa et al., 2011). In response to increased pressures on water resources due to more intense droughts, the use of reclaimed wastewater in agricultural irrigation has been suggested to be increased in Europe (e.g., Nikolaou et al., 2020; EU Regulation 2020/741). While beneficial for helping to ease water stress, reclaimed wastewater can contain a myriad of anthropogenic chemicals (such as pharmaceuticals and personal care products; e.g., Ben Mordechay et al., 2018) and so its increased use could result in increased emissions of these chemicals to agricultural environments. With the push towards a circular economy, nutrient recycling through biosolid application to agricultural fields may increase (e.g., EC, 2020), resulting in increased availability of the anthropogenic chemicals (such as pharmaceuticals) and microplastics present in biosolids for human exposure through the agricultural food chain (e.g., Tavazzi et al., 2012; Corradini et al., 2019; Ben Mordechay et al., 2018).

Chemical persistence and formation of transformation products in the environment is also likely to be changed by a range of global change drivers. Current approaches for assessing chemical persistence from a regulatory perspective require that persistence tests be conducted at the mean surface water temperature of Europe of 12°C (ECHA, 2017). These persistence data are then extrapolated to different temperature conditions using the Arrhenius equation (FOCUS, 2006). However, the log-linear extrapolation used by the Arrhenius equation may not be valid for higher temperatures (e.g., extrapolations from 12°C to 30-40°C; see Meynet et al., 2020). Furthermore, understanding of transformation products of chemicals occurring from biodegradation, and the physicochemical properties of these transformation products, is generally limited (e.g., González-Gaya et al., 2021). Changes in soil microbial communities in concert with climate change and other global changes could also impact these chemical transformation products.

Chemical fate and transport will also likely be impacted by global change. Chemical mobilization from agricultural fields has been shown to be tied to intense precipitation events (e.g., Camenzuli et al., 2012; Yang et al., 2012). The projected increased intensity of rainfall events under climate change (e.g., EEA, 2017) may change the dynamics of chemical mobilization from agricultural fields. Conversely, with projected increased frequency and duration of droughts (e.g., EEA, 2017), a general increase in the time between precipitation events may have impacts on chemical fate and transport, the dynamics of which are poorly understood (Ademollo et al., 2011; see also Ribarova et al., 2008). Furthermore, increased intensity of heatwaves under climate change would enhance the volatilization of chemicals from agricultural fields (e.g., Bloomfield et al., 2006), thus impacting their atmospheric transport (however the balance between increased degradation with increased volatilization would vary depending on chemicals properties; e.g., Wöhrnschimmel et al., 2013). In addition to these changes, shifts in agricultural irrigation techniques to enable increased water usage efficiency (Nikolaou et al., 2020) would impact the route of entry of chemical contaminants in the water into the environment if reclaimed wastewater is being used, potentially impacting chemical fate and transport (e.g., Narain-Ford et al., 2020).

Description of Planned Approach:

Despite the many possible impacts of global change on how chemicals may enter and move in watersheds impacted by urban and agricultural activities in the coming decades, prospective, holistic exposure assessments in the context of the identified global change drivers are lacking. In this deliverable, we identify modelling frameworks that will be used in the forthcoming deliverable that our Work Package will provide (i.e., D4.4, "Future ecological and human exposure scenarios"), that address the following question:

How will concentrations of anthropogenic chemicals (namely those coming from urban and agricultural areas) change in surface water in the coming decades, and how will this impact chemical exposures of aquatic species, and humans through consumption of drinking water & fish?

To address this question, we plan to use a suite of existing chemical fate, transport, and exposure models at varying spatial and temporal scales to forecast how the interconnected elements of global change may impact chemical exposure. The four existing models identified as suitable for this purpose are the SimpleTreat model (Struijs, 2014), RAIDAR (e.g., Arnot et al., 2006), BETR-Global (MacLeod et al., 2011), and ACC-HUMAN (Czub and McLachlan, 2004).

SimpleTreat is a non-equilibrium, steady state mass balance model used to estimate the fate of down-the-drain chemicals within wastewater treatment plants, and is used within the European Union's Registration, Evaluation, Authorization, and restriction of Chemicals (REACH) legislation. The model takes estimates of down-the-drain chemical emissions, chemical properties, and wastewater treatment plant operating details and calculates the partitioning of chemicals present in the influent sewage to the outgoing liquid effluent, the solid sludge, chemical emissions to air, and chemical degradation within the treatment plant (Struijs, 2014). SimpleTreat has been used at the watershed scale to estimate emissions of anthropogenic chemicals to surface water bodies due to wastewater treatment plant effluent release (e.g., Douziech et al., 2018; Kilgallon et al., 2017).

The Risk Assessment Identification and Ranking (RAIDAR) model is a screening-level chemical fate, exposure, bioaccumulation, and risk assessment model that provides estimates of risk posed to the most sensitive species in an evaluative regional environment (e.g., Arnot et al., 2006; Arnot and Mackay, 2008). Within the screening framework, chemical property data and estimates of emissions are input, along with effect concentrations of the compounds. A unit emission is assumed for each chemical, and the chemical fate and transport within the abiotic environment is then calculated within a Level II (steady-state, equilibrium) or Level III (steady-state, non-equilibrium) framework. Bioaccumulation through aquatic and terrestrial food webs are then calculated, and the highest exposure concentration to effect concentration ratio is identified throughout the modelled species to identify the most sensitive organism. The user-input emission rate can then be compared to the modelled unit emission rate to determine the risk that may be posed from the estimated amount of chemical entering the environment. This screening-level modelling framework identifies chemicals of greatest concern that can then be assessed using more comprehensive environmental exposure and risk modelling methods that incorporate more site-specific realism (Arnot et al., 2006). RAIDAR has been used in high-throughput chemical risk assessment in Canada and is part of the human exposure modelling suite of tools within the US EPA's ExpoCast System (see ARC, 2021; US EPA, 2021).

BETR-Global is a multimedia, fugacity-based, steady-state or dynamic, mass-balance model used to simulate the fate and transport of persistent organic pollutants globally (e.g., MacLeod et al., 2011). Using a spatial grid with user-selected cell sizes (e.g., 15^{o} or 3.75^{o} latitude/longitude), BETR-Global takes as input chemical emission amounts to 7 different environmental media (lower atmosphere, upper atmosphere, vegetation, soil, freshwater, freshwater sediments, and ocean water). Environmental conditions parameterized into the model (e.g., precipitation, atmospheric circulations, ocean transport, etc.) along with chemical properties (e.g., air-water and water-lipid partition coefficients, degradation half-lives, etc.) dictate how the modelled chemical moves through each environmental media and between the grid cells of the global model. The model outputs either steady-state or time-dependent concentrations of the chemical in each environmental media in each global grid cell. BETR-Global has been used extensively to model a wide range of chemicals, such as PCBs (e.g., McLachlan et al., 2018), PFOA (Armitage et al., 2009), as well as chemicals over a wide chemical property space (Gouin et al., 2013).

ACC-HUMAN is a fugacity-based dynamic model used to estimate the bioaccumulation of hydrophobic chemicals in humans (Czub and McLachlan, 2004). Biomagnification of the chemical is modelled through an aquatic food chain (through the pathway: water -> zooplankton -> fish -> humans) and an agricultural food chain (through the pathway air/soil -> grass -> cattle -> humans), while also considering human exposure through air and drinking water. Abiotic concentrations of the chemical in the relevant environmental media are fed into the model, along with parameterizations of the food chain and human ingestion amounts. Chemical properties and bioaccumulation parameters throughout the food chains are then employed to estimate human exposure to and bioaccumulation of the modelled chemical, considering either steady-state or dynamic conditions. ACC-HUMAN has been employed in concert with the BETR-Global model to estimate historical bioaccumulation of and human exposure to PCBs (McLachlan et al., 2018) as well as to explore the impacts of possible shifts of dietary trends on human exposure to PCBs in China (Zhao et al., 2018).

The use of these models in different configurations will enable assessment of future scenarios of exposure at a range of spatial and temporal scales, and these configurations are outlined in Table 1.

Table 1. Model configurations to be used in prospective chemical exposure assessments in support of Deliverable D4.4

Model Configuration	**Spatial Scale**	**Chemical Emissions Route**	**Exposure Target**	**Temporal Scale**
SimpleTreat + RAIDAR	Regional	Down-the-drain (surface water)	Ecological + Human	Steady-state
SimpleTreat + BETR-Global + ACC-HUMAN	Global	Down-the-drain (surface water)	Fish + Humans	Steady-state + Dynamic
BETR-Global + ACC-HUMAN	Global	Land/Air	Fish + Humans	Dynamic

Within these modelling frameworks, we will explore the effects on chemical exposure of combined scenarios of changes in pesticide emissions, changes in down-the-drain chemical emissions and contamination of effluent wastewater and biosolids, and changes in the increased use of wastewater for irrigation and the use of biosolids in agriculture. All of these scenarios will be combined with scenarios for climate change, using environmental conditions output from IPCC modelling reports (e.g., IPCC, 2021). Furthermore, given the uncertainties around what chemicals will be used in the future, a wide chemical property space may be analysed, and/or exemplar compounds may be selected for focused analysis.

Summary:

Global change is likely to impact how chemicals are emitted into watersheds impacted by urban and agricultural activities, and climate change specifically is likely to impact the fate and transport processes of these chemicals once they are in the environment. Based on a review of existing literature, we have identified knowledge gaps in understanding of how these global changes will impact the exposure of humans and other species to these chemicals. To begin filling these knowledge gaps, we have identified key aspects of environmental scenarios that need to be explored to constrain exposures under global change conditions. A suite of existing models (i.e., SimpleTreat, RAIDAR, BETR-Global, & ACC-HUMAN) can be parameterized with the projected environmental conditions to explore scenarios of chemical emissions and subsequent exposure. This modelling framework will support the completion of Deliverable D4.4 ("Future ecological and human exposure scenarios for chemical contaminants"), help build understanding related to how elements of global change may impact environmental chemical risk, and potentially elucidate chemical risk mitigation opportunities within the ECORISK Work Package 6 (i.e., "Risks and mitigation").

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Much of this report is synthesized from parts of a manuscript that is currently in preparation based on the outcomes of the ECORISK Deliverable D2.5 (D15): "Workshop on chemical risk in the future", which was an online writing workshop hosted by ECORISK in September-October of 2020. This manuscript is being authored by the following members or affiliates of ECORISK:

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References:

Ademollo, N., Capri, S., Patrolecco, L., Puddu, A., Polesello, S., Rusconi, M., Valsecchi, S., Froebrich, J., 2011. Fate and monitoring of hazardous substances in temporary rivers. TrAC - Trends Anal. Chem. 30, 1222–1232. https://doi.org/10.1016/j.trac.2011.05.002

ARC, 2021. RAIDAR [WWW Document]. URL https://arnotresearch.com/RAIDAR/ (accessed 10.7.21).

Armitage, J.M., MacLeod, M., Cousins, I.T., 2009. Modeling the global fate and transport of perfuorooctanoic acid (PFOA) and perfluorooctanoate (PFO) emitted from direct sources using a multi-species mass balance model. Environ. Sci. Technol. 43, 1134–1140. https://doi.org/10.1021/es802900n

Arnot, J.A., Mackay, D., 2008. Policies for chemical hazard and risk priority setting: Can persistence, bioaccumulation, toxicity, and quantity information be combined? Environ. Sci. Technol. 42, 4648–4654. https://doi.org/10.1021/es800106g

Arnot, J.A., Mackay, D., Webster, E., Southwood, J.M., 2006. Screening level risk assessment model for chemical fate and effects in the environment. Environ. Sci. Technol. 40, 2316–2323. https://doi.org/10.1021/es0514085

Ben Mordechay, E., Tarchitzky, J., Chen, Y., Shenker, M., Chefetz, B., 2018. Composted biosolids and treated wastewater as sources of pharmaceuticals and personal care products for plant uptake: A case study with carbamazepine. Environ. Pollut. 232, 164–172. https://doi.org/10.1016/j.envpol.2017.09.029

Bloomfield, J.P., Williams, R.J., Gooddy, D.C., Cape, J.N., Guha, P., 2006. Impacts of climate change on the fate and behaviour of pesticides in surface and groundwater-a UK perspective. Sci. Total Environ. 369, 163–177. https://doi.org/10.1016/j.scitotenv.2006.05.019

Bruinsma, J., 2009. The Resource Outlook to 2050: By How Much do Land, Water and Crop Yields Need to Increase by 2050?, FAO. https://doi.org/10.1007/978-3-642-41714-6_180309

Camenzuli, L., Scheringer, M., Gaus, C., Ng, C.A., Hungerbühler, K., 2012. Describing the environmental fate of diuron in a tropical river catchment. Sci. Total Environ. 440, 178–185. https://doi.org/10.1016/j.scitotenv.2012.07.037

Corradini, F., Meza, P., Eguiluz, R., Casado, F., Huerta-Lwanga, E., Geissen, V., 2019. Evidence of microplastic accumulation in agricultural soils from sewage sludge disposal. Sci. Total Environ. 671, 411–420. https://doi.org/10.1016/j.scitotenv.2019.03.368

Czub, G., McLachlan, M.S., 2004. A food chain model to predict the levels of lipophilic organic contaminants in humans. Environ. Toxicol. Chem. 23, 2356–2366.

Delcour, I., Spanoghe, P., Uyttendaele, M., 2015. Literature review: Impact of climate change on pesticide use. Food Res. Int. 68, 7–15. https://doi.org/10.1016/j.foodres.2014.09.030

Douziech, M., van Zelm, R., Oldenkamp, R., Franco, A., Hendriks, A.J., King, H., Huijbregts, M.A.J., 2018. Estimation of chemical emissions from down-the-drain consumer products using consumer survey data at a country and wastewater treatment plant level. Chemosphere 193, 32–41. https://doi.org/10.1016/j.chemosphere.2017.11.009

EC, 2020. A new Circular Economy Action Plan for a cleaner and more competitive Europe.

ECHA, 2017. Guidance on information requirements and chemical safety assessment Chapter R . 7b : Endpoint specific guidance November 2012. Eur. Chem. Agency. https://doi.org/10.2823/84188

EEA, 2017. Climate change, impacts and vulnerability in Euopre 2016. Luxembourg. https://doi.org/10.2800/534806

EUROSTAT, 2021. Population projections: urban growth, rural decline [WWW Document]. URL https://ec.europa.eu/eurostat/web/products-eurostat-news/-/ddn-20210520-1 (accessed 10.7.21).

FOCUS, 2006. Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration.

González-Gaya, B., Lopez-Herguedas, N., Bilbao, D., Mijangos, L., Iker, A.M., Etxebarria, N., Irazola, M., Prieto, A., Olivares, M., Zuloaga, O., 2021. Suspect and non-target screening: The last frontier in environmental analysis. Anal. Methods 13, 1876–1904. https://doi.org/10.1039/d1ay00111f

Gouin, T., Armitage, J.M., Cousins, I.T., Muir, D.C.G., Ng, C.A., Reid, L., Tao, S., 2013. Influence of global climate change on chemical fate and bioaccumulation: The role of multimedia models. Environ. Toxicol. Chem. 32, 20–31. https://doi.org/10.1002/etc.2044

Hader, J.D., Lane, T., Boxall, A.B.A., Macleod, M., Di Guardo, A., Enabling prospective assessment of environmental exposure to chemicals in European agriculture under global change. In Prep.

IPCC, 2021. Assessment Report 6 Climate Change 2021: The Physical Science Basis.

Kilgallon, J., Franco, A., Price, O.R., Hodges, J.E.N., 2017. Application of a spatially resolved model to contextualise monitoring data for risk assessment of down-the-drain chemicals over large scales. Environ. Pollut. 230, 954–962. https://doi.org/10.1016/j.envpol.2017.07.041

MacLeod, M., Von Waldow, H., Tay, P., Armitage, J.M., Wöhrnschimmel, H., Riley, W.J., McKone, T.E., Hungerbuhler, K., 2011. BETR global - A geographically-explicit global-scale multimedia contaminant fate model. Environ. Pollut. 159, 1442–1445. https://doi.org/10.1016/j.envpol.2011.01.038

McLachlan, M.S., Undeman, E., Zhao, F., MacLeod, M., 2018. Predicting global scale exposure of humans to PCB 153 from historical emissions. Environ. Sci. Process. Impacts 20, 747–756. https://doi.org/10.1039/c8em00023a

Meynet, P., Davenport, R.J., Fenner, K., 2020. Understanding the Dependence of Micropollutant Biotransformation Rates on Short-Term Temperature Shifts. Environ. Sci. Technol. 54, 12214–12225. https://doi.org/10.1021/acs.est.0c04017

Narain-Ford, D.M., Bartholomeus, R.P., Dekker, S.C., van Wezel, A.P., 2020. Natural Purification Through Soils: Risks and Opportunities of Sewage Effluent Reuse in Sub-surface Irrigation. https://doi.org/10.1007/398_2020_49

Nikolaou, G., Neocleous, D., Christou, A., Kitta, E., Katsoulas, N., 2020. Implementing Sustainable Irrigation in Water-Scarce Regions under the Impact of Climate Change. Agronomy 10, 1120. https://doi.org/10.3390/agronomy10081120

Ribarova, I., Ninov, P., Cooper, D., 2008. Modeling nutrient pollution during a first flood event using HSPF software: Iskar River case study, Bulgaria. Ecol. Modell. 211, 241–246. https://doi.org/10.1016/j.ecolmodel.2007.09.022

Sjerps, R.M.A., ter Laak, T.L., Zwolsman, G.J.J.G., 2017. Projected impact of climate change and chemical emissions on the water quality of the European rivers Rhine and Meuse: A drinking water perspective. Sci. Total Environ. 601–602, 1682–1694. https://doi.org/10.1016/j.scitotenv.2017.05.250

Struijs, J., 2014. SimpleTreat 4.0: a model to predict fate and emission of chemicals in wastewater treatment plants.

Tavazzi, S., Locoro, G., Comero, S., Sobiecka, E., Loos, R., Gans, O., Ghiani, M., Umlauf, G., Suurkuusk, G., Paracchini, B., Cristache, C., Fissiaux, I., Riuz, A.A., Gawlik, B.M., 2012. Occurrence and levels of selected compounds in European sewage sludge samples (FATE SEES). https://doi.org/10.2788/67153

The European Parliament and the Council, 2020. Regulation (EU) 2020/741, Minimum requirements for water reuse. Off. J. Eur. Union 177, 32–55.

US EPA, 2021. Rapid Chemical Exposure and Dose Research [WWW Document]. URL https://www.epa.gov/chemical-research/rapid-chemical-exposure-and-dose-research (accessed 10.7.21).

Van Der Aa, N.G.F.M., Kommer, G.J., Van Montfoort, J.E., Versteegh, J.F.M., 2011. Demographic projections of future pharmaceutical consumption in the Netherlands. Water Sci. Technol. 63, 825–831. https://doi.org/10.2166/wst.2011.120

Wöhrnschimmel, H., Macleod, M., Hungerbuhler, K., 2013. Emissions, fate and transport of persistent organic pollutants to the arctic in a changing global climate. Environ. Sci. Technol. 47, 2323–2330. https://doi.org/10.1021/es304646n

Yang, Y.Y., Gray, J.L., Furlong, E.T., Davis, J.G., Revello, R.C., Borch, T., 2012. Steroid hormone runoff from agricultural test plots applied with municipal biosolids. Environ. Sci. Technol. 46, 2746–2754. https://doi.org/10.1021/es203896t

Zhao, S., Breivik, K., Jones, K.C., Sweetman, A.J., 2018. Modeling the Time-Variant Dietary Exposure of PCBs in China over the Period 1930 to 2100. Environ. Sci. Technol. 52, 7371–7379. https://doi.org/10.1021/acs.est.8b01228