https://www.canada.ca/en/health-canada/services/chemical-substances/chemicals-management-plan/science-committee/meeting-records-reports/objectives-paper-june-12-13-2019.html

Objectives paper - June 12–13, 2019

Chemicals Management Plan Science Committee

New approaches for integrating chemical **f**ate and spatial and temporal scale in exposure assessment

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- Appendix 2: Basics for local predicted environmental concentration (PEC) calculations

1.0 Introduction

1.1 The issue

Estimating media concentrations of chemicals in the environment adds an important source of uncertainty to chemical risk assessments. Largely, this stems from the variable and dynamic nature of environmental conditions, chemical fate, and chemical emissions. Most environmental concentrations used for ecological risk assessments in the Chemicals Management Plan (CMP) are based on local-scale scenarios, while local- and/or regional-scale scenarios are considered for human health risk assessments. More specifically, in many instances there is currently limited consideration of how emission rate, fate, and transport quantitatively affect exposure to human and non-human receptors beyond the local scale. Essentially, the potential for exposure at the regional and far-field scales is not routinely considered in ecological exposure assessment conducted by the Government of Canada (GoC) within the context of the CMP. Bonnell et al. (2018) suggest that one reason for this is the limited integration of chemical fate and distribution information when estimating environmental concentrations, particularly beyond point-source emission areas. This can result in a spatial and temporal mismatch between the environmental concentrations driving prioritization or risk assessment and actual or anticipated exposures. This challenge has also been identified by the National Academy of Sciences (NAS) report "Using 21st Century Science to Improve Risk-Related Evaluations" (NAS, 2017).

"*Improve Knowledge of Processes that Determine Chemical Fate in Systems. Challenge: Understanding the influence of processes that control the fate, transport, and ultimately concentrations of chemicals in environmental compartments and in animal and cell-based test systems is essential for characterizing and predicting exposures. Information on system properties, processes, and transformation pathways that contribute to chemical exposure is nonexistent, incomplete, and inconsistent, and this limits the capacity for more comprehensive, quantitative exposure-based and risk-based evaluations*". (NAS, 2017)

The 2017 NAS report recommends that databases for chemical properties, transformation rates, and pathways should be developed to support the development of exposure science. It further emphasizes the role of predictive computational approaches to improve exposure science for risk-based assessments given that few exposure measurements are available for the vast majority of environmental stressors (NAS 2017). The NAS report also highlights that "the recognized absence of tools and exposure information is stimulating research to improve near field and far field exposure science" (NAS, 2017).

The use of local-scale scenarios typically represents a "worst case," which can be desirable as it is a conservative approach from a risk assessment perspective. However, in CMP risk assessments there can be a need to refine such exposure estimates (for example, in cases where there is a narrow margin between the estimate of exposure and the hazard point of departure). Expanding the exposure scenario beyond the local scale provides an opportunity to consider real-world factors that would potentially impact the exposure of target receptors. The GoC therefore seeks to better integrate chemical fate and spatial and temporal scale of exposure in an effort to improve the quantitative estimation of multimedia exposure beyond the local scale, considering dynamic (episodic, non-steady state) as well as steady-state emission conditions. Such quantification of exposure would result in refined, more realistic exposure scenarios and predicted environmental concentrations, and increased accuracy in the estimation of risk. The integration of chemical fate and the spatial and temporal scale would decrease uncertainty in exposure assessment, increase confidence in CMP risk assessments conclusions, and ultimately aid in the decision-making process in chemical risk management. This integration would also benefit subsequent risk management and pollution prevention efforts because the efficacy of emission reductions can be better understood across spatial and temporal scales as well as including sensitive remote locations, which may affect various vulnerable populations (for example, MacKay and Reid, 2008). In order to understand how connections across these scales of exposure can be made, however, an understanding of emission patterns and chemical fate (including persistence) is needed.

1.2 Chemicals Management Plan Science Committee objective and topic context

The objective of the CMP Science Committee (SC) topic is to seek feedback on areas where exposure assessment could be further refined to better integrate chemical fate and varying spatial and temporal scales of exposure. This topic is focused on environmental exposures of humans and other organisms, but it does not include human exposure from consumer products or indoor air. Human exposures to chemicals from consumer products and indoor air have their own complexities and challenges and, for the purpose of achieving a suitable focus for this SC discussion, will be excluded. Output from this topic may inform risk assessment and/or management activities by the GoC within the context of the current CMP, but may also inform future prioritization and assessment activities (for example, post 2020). Previously, Environment and Climate Change Canada's (ECCC's) Ecological Risk Classification (ERC) approach incorporated multimedia fate and qualitative spatial scale of exposure. Human exposures from environmental media have been estimated using a multimedia fate model in CMP assessments. The GoC recognizes that this issue can become complex and involve complex tools. Therefore, it is desirable that the SC discuss approaches that are "fit-for-purpose" for CMP evaluation needs, perhaps involving a tiered structure for implementation.

Much of the discussion on this topic will involve new approaches or adaptations of current approaches to fate and exposure modelling, given that the majority of prioritization and a significant proportion of risk assessment conducted by the GoC occur in the absence of monitoring data.

It is not the intention of this document to provide an extensive review of all available models or approaches, which are described in the literature (for example, OECD, 2004; Zhang et al., 2012). This document discusses some current GoC approaches and needs for improved integration of chemical fate and spatial and temporal scales for environmental exposure assessment. As such, there is a focus on environmental fate modelling of discrete organic chemicals, which includes ionizing organic chemicals but excludes inorganic substances, polymers, and truly complex unknown or variable composition, complex reaction products, and biological materials (UVCBs).[1] There are additional uncertainties and/or data gaps currently associated with the estimation of environmental media concentrations for these substances that could not reasonably be addressed here. Assessing the exposure of degradation products remains within the scope of this topic, provided that some knowledge of the degradation product is available for modelling purposes (for example, on structure, physical, and chemical properties; persistence). Finally, while this topic has a focus on

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[1] Where a UVCB cannot be suitably represented by a discrete chemical structure.

environmental modelling, conceptually it is also applicable when planning monitoring programs. Current and future monitoring can scale from near field to far field in accordance with modelled chemical fate, and conversely, the results of monitoring can improve fate and exposure modelling.

The following sections provide a GoC perspective of fate and exposure assessment under the CMP as well as related scientific concepts to aid the SC when examining the charge questions. A descriptive summary of a generic local-scale approach and predicted environmental concentrations (PECs) used by the GoC for environmental risk assessment for both new and existing substances is provided in Appendix 1 and 2, respectively.

2.0 Definitions

For the purposes of this document, the following definitions will be used to describe key concepts for this topic.

- advection: bulk transport of a chemical in water or air out of the regional-scale multimedia model environment (based on Mackay et al., 1996a)

- characteristic travel distance (CTD)*:* the distance at which the concentration of a chemical in air or water is reduced to 63% from degradation and partitioning to other media (based on Bennett et al., 1998; Beyer et al., 2000)

- clearance time, lag time, response time: the time (hours) required to reduce the mass of chemical in the environment by a specified percentage (for example, 50%, 95%) once all emissions have ceased, as determined by using a multimedia model (based on Stroebe et al., 2004; Gouin and Wania, 2007)

- continental scale (far field)*:* exposures distant from points of emission (for example, polar regions, intercontinental distances, transboundary), typically >1,000 km [based on van de Meent (1993) and MacKay, et al. (2014)]

- continuously present: a constant exposure to chemicals continuously emitted to the environment where the time to exposure is less than the time to degrade (based on

MacKay et al., 2014). This term is preferred over "pseudo-persistence" (Daughton, 2002) to avoid confusion over its relationship as an intensive property of a substance

- local scale (near field): exposures relatively close to the source of emission or discharge (for example, close proximity to the end of a sewage treatment pipe, indoor air) [based on van de Meent (1993)[2] and MacKay et al. (2014)]

- mode of entry: whether a chemical is released to water, air, or soil (based on OECD, 2004)

- overall persistence: sum of all medium-specific half-lives (hours) of a chemical weighted according to the mass fraction of the chemical in a medium (based on Pennington, 1997)

- realistic presence: avoiding undue consideration of the exposure of a chemical when the mass fraction (percent) in a medium is not significant (for example, <5%) (based on Woodfine and Mackay, 2001)

- regional scale *(regional field):* exposures up to moderate distances (for example, within few hundreds of kilometers) from points of emission, and typically defined in mass balance multimedia models as being within a 100,000-km^2 region [based on van de Meent (1993) and MacKay et al. (2014)]

- residence time: a multimedia model estimate of the time (hours) a chemical resides in the environment, considering loss of the chemical from degradation (reaction) and advection (transport) out of the model environment. It is sometimes used synonymously with overall persistence (Pov), which ignores loss from advection (for example, OECD, 2004)

3.0 Emission pattern

The predicted environmental concentration (PEC) used in environmental exposure assessment at the local scale is arguably most sensitive to emission pattern and mode of entry (see section 4.2.1). These parameters contribute to one of the largest sources of

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[2] Noting that van de Meent (1993–2014) includes a personal scale for human occupational exposures.

uncertainty in risk assessment because they are currently not well characterized (for example, due to a lack of downstream use data post-manufacture or post-import), and estimated PECs tend to be comparatively uncertain. For example, future chemical tonnage and use pattern forecasting (long-term, >3 years) or aggregation of emissions (and scenarios) is not routinely performed in exposure assessment. Once a chemical is listed on Canada's Domestic Substances List (DSL), except in some specific instances it may be used for any purpose at any tonnage. This ultimately leads to the most current CMP exposure assessment that represents a "snapshot" of current emissions for specific exposure pathways that are generally assumed not to change over time and space. Appendix 1 provides further details on parameters and assumptions used in generic local emission models used by ECCC and HC, including chemical tonnage reporting and selection, emission factors, and rates.

If knowledge of the temporal emission pattern (for example, episodic vs. continuous) is available, the time between release intervals is used to select ecotoxicity values (acute for episodic, chronic for continuous) for the ecological hazard evaluation [similar to the European Union System for the Evaluation of Substances (EUSES) guidance; see section 4.1]. The impact of residence time on exposure to a chemical (see section 4.3) is typically not factored into this decision.

Different approaches may be used for determining spatial emission patterns, which depend on the substance being assessed and on the reported use patterns. These approaches include:

1. selection of a single representative site (for example, in the case of substances that have very specialized applications and are expected to be used by a limited number of facilities, with no realistic expectation of a substantial market change)
2. selection of multiple representative sites (typically not aggregated)
3. use of distributions of parameter(s) to represent a sector (semi-probabilistic or probabilistic approaches)[3]

Exposure resulting from different life-cycle stages is considered to the extent possible. Key stages often include manufacture, formulation, industrial use, service life, and sometimes end

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[3] For instance, if a substance is broadly used within a chemical sector (for example, lubricant additive), a distribution of flow rates from receiving water bodies associated with facilities in this sector is generated. A conservative value distribution (for example, 10th percentile) is then taken for exposure calculations.

of life. The selection of relevant life-cycle stages is determined based on the available data and identification of likelihood of release. Not all industrial sectors or activities identified necessarily require quantitative release characterization. Quantification depends on the tonnages, potential for release, and data availability.

4.0 Integrating chemical fate

4.1 The impact of Domestic Substances List (DSL) categorization on chemical fate assessment

The assessment of chemical fate has been a fundamental part of *Canadian Environmental Protection Act*, *1999* (CEPA 1999) risk assessment since the 1990s [for example, Priority Substance List (PSL) assessments). Decades ago, the evaluation of chemical fate was mainly done qualitatively based on the physical and chemical properties of a substance, as well as monitoring results from various environmental media, when available. Some PSL substance assessments included fate modelling, but it was not standard practice. In Canada, at the start of the millennium, a paradigm shift to rapid assessment of substances based largely on "hazard properties" (for example, persistence, bioaccumulation, and median lethal ecotoxicity) occurred in which the combination of persistence and bioaccumulation acted as a surrogate for fate (and exposure) for both new and existing substances. The 1995 Toxic Substances Management Policy (TSMP) document states the following:

> Exposure is an important element in evaluating environmental risk under the policy. Persistence and bioaccumulation can be used as qualitative surrogates for long-term exposure of environmental biota.

Categorization of the DSL for both ecological and human exposures and a large part of the first phase of the CMP (the "Challenge" Initiative) relied on these properties (that is, persistence and bioaccumulation) as surrogates for fate and environmental exposure assessment. However, the hazard property approach, while still important as a precautionary assessment of exposure for situations where exposure quantification is not possible or highly uncertain, reduced the fate component of the assessment to the determination of key physical and chemical properties. A consequence is that this approach may not adequately address exposure in many circumstances, and would not be relevant in certain situations (for example, when exposure can be quantified). For example, inherently toxic substances that are neither highly persistent nor bioaccumulative (for example, ionizing chemicals) but are continuously discharged to the environment would not be adequately captured by this approach. High-tonnage substances that come close to but do not meet or exceed Canadian persistence and bioaccumulation criteria (Canada, 2000) would not be well captured by this approach, either. Further, the hazard property approach may also target substances with a low potential for environmental exposure (for example, low tonnage chemicals), which would not be of concern, resulting in a significant impact on chemical management plans and resources. A further implication is that because the “hazard mindset” has become somewhat pervasive when considering chemical fate and exposure, less development of exposure science has occurred globally.

4.2 Multimedia fate modelling in the Chemicals Management Plan (CMP)

4.2.1 General evaluative fate models

CEPA 1999 ecological risk assessments in the last 10–12 years have returned to being risk driven, where more detailed fate and exposure assessments are considered. Typically, for organic chemicals, fate assessment has involved the application of generic multimedia fate models to determine basic media partitioning and distribution as well as long-range transport (LRT) in air. More recently, LRT in water has been considered in ecological assessments because priority substance chemistries have shifted from the traditional hydrophobic persistent organic pollutants (POPs) to include several classes of ionizing chemicals under the third phase of the CMP. Generic regional-scale fate models employed by the GoC are “MacKay-type” models, including the Equilibrium Criterion Model (EQC) (Mackay et al., 1996a, b) and a Canadian ecozone version of the EQC model known as ChemCAN (Webster et al. 2003).[4] Mass-balance models are also used to estimate removal by waste treatment systems such as SimpleTreat 3.0 (Struijs, 1996) and the updated Toronto Sewage Treatment Plant (STP) removal model (Seth et al., 2008) integrated into the Unites States (U.S.) Environmental Protection Agency’s (EPA’s) EPIWIN suite.

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[4] Noting that other Mackay type models such as the Biosolids-Amended Soil: Level IV or BASL4 (Hughes et al., 2005) for soil fate modelling are also used.

For environmental exposures within the ecological context, the main function of regional models is to determine the mass fraction distribution of a chemical (percent) in air, water, soil, and sediment according to a specified mode of entry and using a default emission rate (Table 1 and Figure 1). The concept of "realistic presence" (Mackay et al., 2014) is not routinely considered (that is, water concentrations are always derived, even if there is low mass fraction in this medium).

The mode of entry into the environment (that is, air, water, soil) has a significant impact on the mass balance and fate of a chemical because a receiving medium initially contains the largest mass of the chemical and influences the subsequent behaviour and distribution of the chemical. Webster et al. (1998) explain this concept in detail. Ideally, partitioning of the emission rate according to a known mode of entry into the environment (for example, 20% water, 75% soil, 5% air) would represent a more realistic fate and mass balance of the chemical in the environment. Regional-scale fate and environmental concentrations estimated by the model would thus reflect the known mode(s) of entry. However, this is rarely performed as described under the CMP for ecological assessments because a detailed knowledge of use pattern (for example, downstream use) is generally not available.[5] Advective inflows or background concentrations of the substance from air and water are taken into consideration if available (or can be estimated), but this is not usually done when regional-scale models are used in ecological assessments.

Mass-balance models require physical and chemical properties and media half-life information to simulate fate and exposure at a regional scale (see section 3.0). As a consequence of having a local-scale focus in the CMP (particularly in ecological assessments), mass-balance models are not generally used for environmental concentrations in CMP risk assessments. There are some exceptions to this; notably, dispersed environmental concentrations estimated using a regional-scale mass-balance model (ChemCAN) are often used to estimate exposures of the Canadian general population to chemicals through environmental media using conservative inputs, and considering all possible modes of entry.

Local-scale environmental concentrations for non-aquatic media are predominantly determined using simple equilibrium partitioning approaches (Appendix 2). The impact of advection (transport) on chemical distribution is often assessed using a mass-balance model, which determines travel distances of chemicals via long-range transport.

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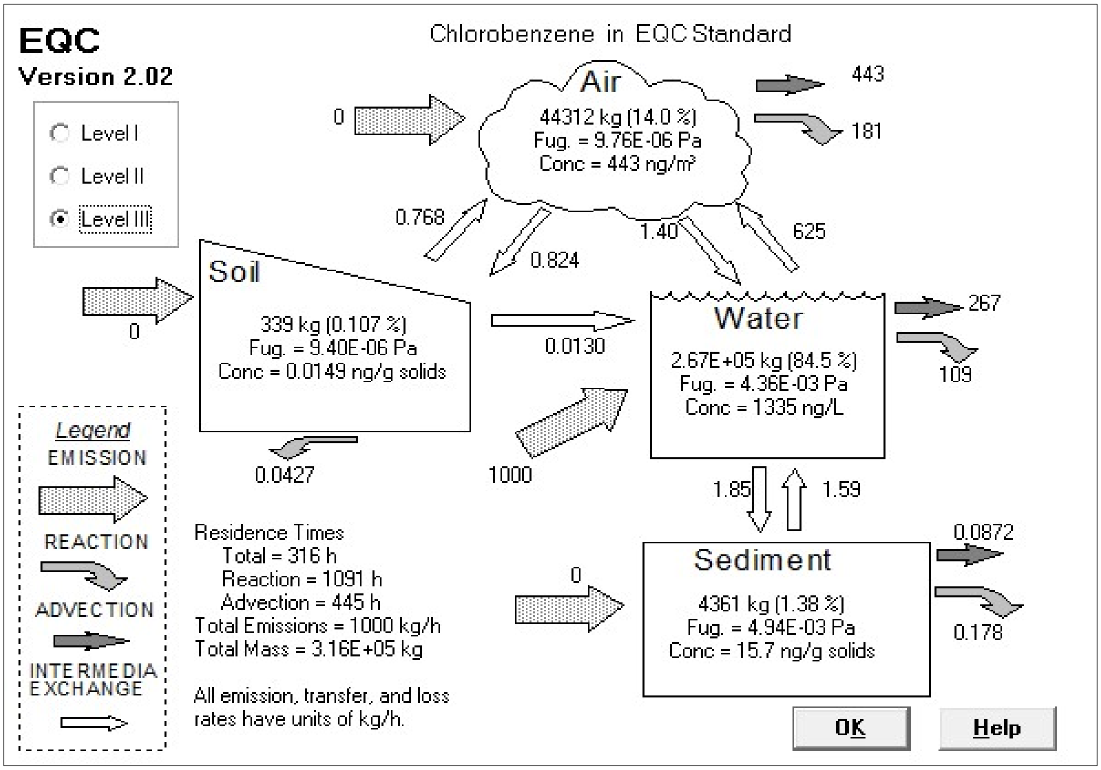
[5] An exception is the cyclic siloxane D5, where mode of entry information was provided to ECCC by industry.

Table 1. Example mass-fraction partitioning results from level III EQC regional model for chlorobenzene using a default emission rate of 1000 kg/hr to air, water, and soil

Substance released to:	Air (%)	Water (%)	Soil (%)	Sediment (%)
Air (100%)	98	1	1	<1
Water (100%)	14	85	<1	1
Soil (100%)	<1	8	92	<1

Figure 1. Example Level III mass-balance output from the EQC Model showing losses due to reaction and advection, and residence time with 100% release to water.



○ Level I
○ Level II
● Level III

Residence Times
Total = 316 h
Reaction = 1091 h
Advection = 445 h
Total Emissions = 1000 kg/h
Total Mass = 3.16E+05 kg

All emission, transfer, and loss rates have units of kg/h.

4.2.2 Long-range transport and regional foodweb modelling

The GoC was part of an extensive review of multimedia fate and transport models and their application in regulatory programs as part of an Organisation for Economic Co-operation and Development (OECD) effort to develop a global model for persistence and long-range transport (OECD, 2004; Wegmann et al., 2008). Chapter 5 of the OECD 2004 document provides useful guidance for the application of multimedia models in regulatory programs, particularly for long-range transport. The Canadian Environmental Modelling Network (CEMN) and Environment Canada also prepared guidance for the application of multimedia fate models specific to GoC programs, which remains useful in this context as well (Webster et al., 2005). The 2004 OECD effort translated into the fairly routine consideration of long-range transport in CMP ecological assessments using the OECD POPs Tool (Wegmann et al., 2008) and the Transport and Persistence Level III (TaPL3) model (Beyer et al., 2000; Webster et al., 2003). These models produce estimates of the “characteristic travel distance or CTD” (km), which are compared to the CTDs of benchmark chemicals for assessment purposes.

Fate in aquatic and terrestrial foodwebs is not routinely characterized in CMP ecological risk assessments noting that, in some cases, exposures to aquatic and terrestrial wildlife using a bioenergetic version of the U.S. EPA wildlife total daily intake models has been performed (for example, brominated flame retardants, substituted diphenyl amines). Coupled environmental fate and foodweb models have been employed in the CMP for ecological prioritization purposes. For example, the regional-scale Risk Assessment, Identification, And Ranking (RAIDAR) model (Arnot et al., 2008) was used to aid rapid screening of DSL chemicals for ecological assessment by the GoC (Environment Canada and Health Canada, 2014). A modified version of RAIDAR was also applied to ionizable chemicals in pharmaceuticals and personal care products on the In Commerce List (ICL) (Arnot, 2011) for Health Canada and most recently for the ecological re-prioritization of 640 organic substances for the third phase of the CMP by ECCC (Arnot, 2014; ECCC, 2016). RAIDAR has the capability of evaluating chemical hazard, exposure, and risk by integrating toxicity, fate, and exposure in a single model, albeit at a regional scale.

4.3 The role of persistence in exposure assessment

Understanding chemical persistence is fundamental to understanding exposure and "is arguably the most important single criterion affecting chemical exposure and risk via the environment" (Mackay et al. 2014). Persistence is directly related to "residence time" and "clearance or lag time" of a chemical in the environment, as well as the mass-fraction distribution of a chemical in various media (Mackay et al., 1996a). Chemicals that degrade slowly can contribute to prolonged exposure, and can potentially be transported long distances in mobile media (air, water, biota). In CMP assessments, a basic assumption is that predicted environmental concentrations reflect steady-state condition emissions and will not change over time. As mentioned earlier, they are thus a "snapshot" of exposure extrapolated over time and space. This assumption is likely appropriate for near-to-source exposures when relatively persistent chemicals are continuously released (the most common assumption in CMP assessments). In this situation, the chemical is considered "continuously present," and it is assumed that the time to exposure is less than the time to degrade regardless of distance from the source. The implication is that all chemicals are treated as if they had a time to exposure greater than a time to degrade, which is not necessarily the case. That is, the exposure concentration is assumed to be homogeneous over a distance (for example, in a flowing river), and media dilution controls exposure. This effectively ignores the role of persistence in exposure evaluation. However, close to the point of release, given a chemical that is continuously present, the persistence of the substance is largely irrelevant because of the short time to exposure. This can be interpreted to mean that "concentrations, exposures, and risk are constant with time, but variable spatially" (Mackay et al. 2014). In instances where the time to exposure is long, the residence time (determined by degradation and advection and dilution) in the environment becomes a major determinant of exposure, particularly at a distance from the source.

Persistence and residence times are also important factors when considering episodic emissions to the environment. If the residence time in hours is much shorter that the interval between episodic emissions (for example, by a factor of 3), each pulse of the chemical can be treated independently, as there is no build-up of the chemical. The exposure pattern in this case becomes "reverse saw-toothed" (that is, exhibits an exposure concentration pattern of spikes and valleys). This is a common outcome, for example, in the exposure scenario of a single biosolids application to agricultural soils. Concentrations of moderately persistent chemicals decline during the year according to their residence time in soil, and then spike again with the next biosolids application. In ecological assessments, acute exposure scenarios (including the use of acute toxicity data) are often considered by regulators for episodic releases. However, when residence time is equal to or longer than the emission interval, then some accumulation of a chemical will occur and concentrations will eventually reach steady state (Mackay et al., 2014). Build-up in non-mobile media such as soil and sediment can become an exposure issue, given that loss of the chemical will be mainly due to natural loss processes such as burial or in some cases volatilization [that is, the residence time is longer than the exposure interval(s)]. Chemical concentrations of highly persistent chemicals gradually increase over time, resulting in long-term exposures higher than those initially predicted based on a single-release event, which may result in an underestimate of risk. Using a regional- or far-field model, increasing concentrations of highly persistent chemicals resulting from (or compounded by) long-range transport can also be estimated. A similar build-up of chemical from episodic emissions can also occur in the far field. The effect of changes in chemical emissions on far-field concentrations as a function of residence time ("distant residence time") is discussed in detail by Mackay and Reid (2008), and Reid and Mackay (2008). The ability to predict the accumulation of persistent (and toxic) chemicals in consideration of the regional- and far-field scale is critical to identifying long-term ecological and human health risk from chemical exposures from the environment.

4.4 Summary and reading

The routine connection of chemical fate with exposure has been somewhat lost in global risk assessment practices because of the impact of the hazard property approach and this impact on the development of integrated fate-exposure tools for risk assessment that represent regional/continental-specific conditions.[6] Emission pattern, mode of entry, partitioning, and persistence all heavily impact how organisms become exposed to chemicals in the environment because they influence residence time in a specific medium or the whole environment. These factors are essential for understanding basic chemical distribution in the environment, and how they directly affect the temporal and spatial scale of exposure. Understanding their influence is vital for determining chemical risk potential over multiple exposure scales (Scheringer et al., 1996; MacKay et al., 2014).

Recommended reading:

- Mackay, D., Di Guardo, A., Paterson, S., Cowan, C.E. 1996a. "Evaluating the environmental fate of a variety of types of chemicals using the EQC model." *Environmental Toxicology and Chemistry*, 15: 1627-1637. Available at https://setac.onlinelibrary.wiley.com/doi/epdf/10.1002/etc.5620150929.
- Mackay, D., Hughes, D. M., Romano, M., and Bonnell, M. 2014. "The role of persistence in chemical evaluations." *Integrated Environmental Assessment and Management*, 10(4): 588–594. Available at https://setac.onlinelibrary.wiley.com/doi/epdf/10.1002/ieam.1545.

5.0 Integrating temporal and spatial scale

In a retrospective analysis of human and ecological exposure assessment approaches, Bonnell et. al. (2018) make several recommendations for new approaches and directions for exposure assessment, including a basic need to better align chemical fate and exposure scale (temporal and spatial) with emission scenarios for deriving predicted environmental concentrations. The authors also point out that one of the reasons for the misalignment is

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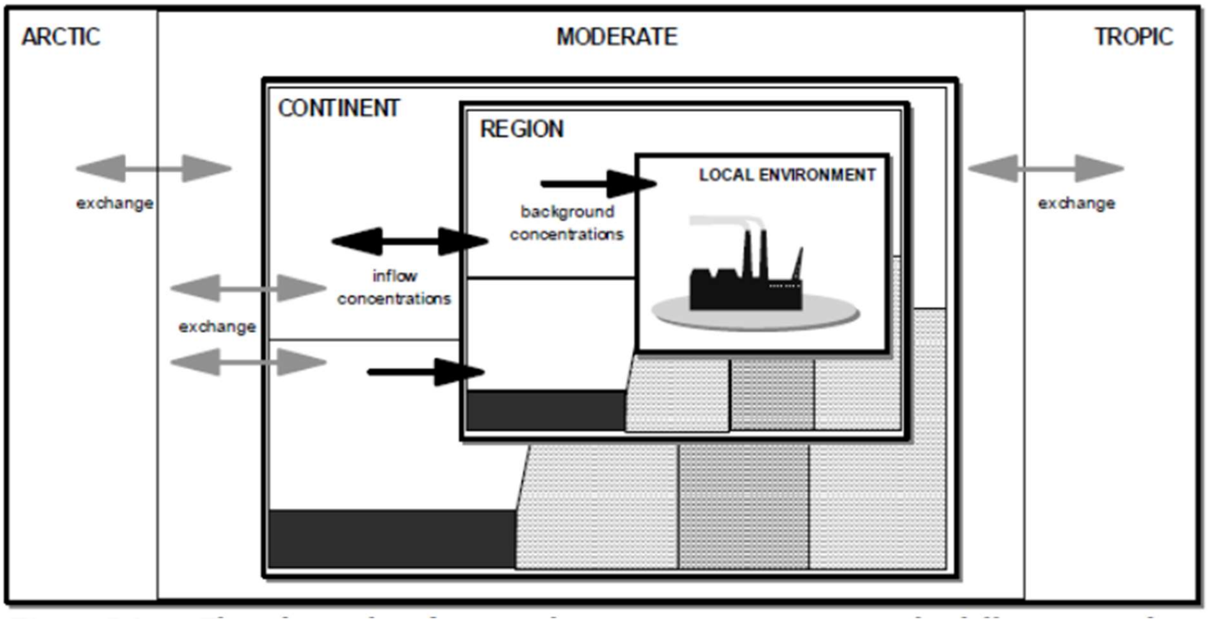
[6] Noting the exception of SimpleBox in European Union System for the Evaluation of Substances (EUSES).

that there are few scalable dynamic multimedia exposure models in existence, and none yet exist that are specific to Canadian environments. As discussed previously, several other tools and approaches are available, which have been used by the GoC to address exposures in various environmental compartments and at various spatial scales, but these are not yet integrated into a single modelling approach.

5.1 Spatial scale

One example of an integrated exposure modelling approach used by a regulatory authority is the European Union System for the Evaluation of Substances or EUSES. EUSES incorporates a “nested” (that is, scaled) multimedia model known as SimpleBox (first version, van de Meent, 1993), which allows the chemical fate and exposure to scale from the local environment to the global scale (Figure 2). EUSES provides a central tool for member countries to estimate environmental exposure concentrations for risk assessments undertaken as part of REACH at various spatial scales. ECHA is currently spearheading a large effort to revise and update the science behind EUSES, which could also benefit the GoC moving forward.

Figure 2. Basic concept of a “nested” multimedia model demonstrated using SimpleBox in EUSES.



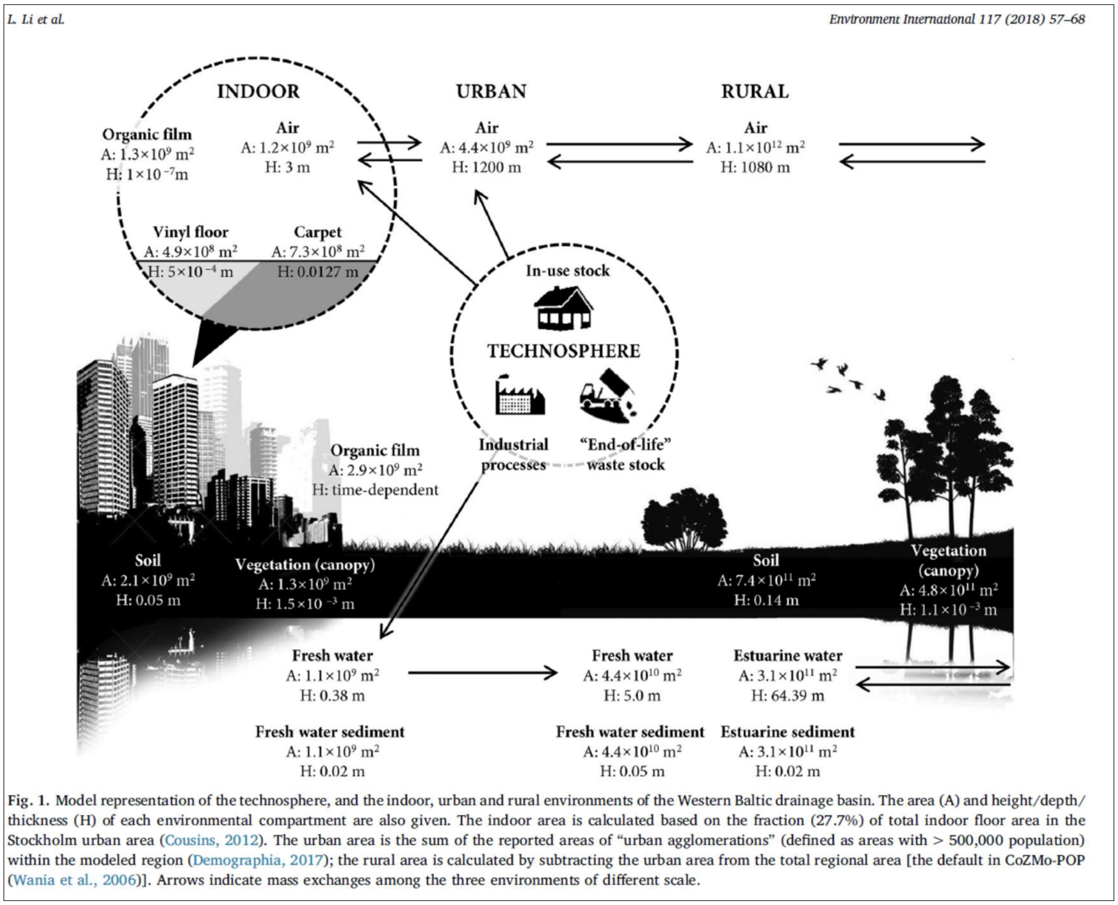
A scaled model such as SimpleBox uses a connected series of environments represented in Figure 2 as local, regional, continental, and global "boxes." The MacKay-type model environments within these boxes are defined similarly to those that exist in other multimedia models such as EQC (with the exception of the local environment). The scaled or nested approach provides a continuum for exposure because chemical flux from one box to another, representing advection and diffusion flow in and out of the box environments, is tracked. The chemical is therefore "not forgotten" from the previous exposure space.

If only local exposures are evaluated, for example, exposures from transport of the chemical to the regional and far field via advection are ignored. Conversely, contributions from the regional and far field to the local scale are also not accommodated (Figure 2). Chemical emissions can be inputted at any scale of the model and, as such, exposures can be aggregated from various points and dispersed sources. As a result, a more representative exposure concentration estimate, at any scale, is generated. Exposure concentration estimates at various scales are derived based on the mass balance within each box, noting that at the local scale, environmental concentrations are not derived based on Mackay-type mass-balance models. These are based on a local-scale model (similar to those used in the CMP) to which concentration estimates from the regional scale are added as background exposures (EUSES, 2004).

SimpleBox is perhaps the first instance of a basic scaled or nested model approach for environmental media. More recently, Fantke et al. (2016) have developed a conceptually similar approach to SimpleBox for human exposure to chemicals from consumer products. This framework was developed to address inter-compartmental transfer fractions of chemicals over various spatial scales between near-field and far-field compartments to ultimately deduce exposure contributions from various pathways and media to intakes by humans (Fankte et al., 2016). The authors suggest that this approach is also useful in determining daily intake fractions for risk assessment and prioritization, as well as alternatives and life-cycle assessment.

Li et al. (2018) developed a multi-scale exposure model conceptually similar to that by Fantke et al. (2016). Neither of these approaches have been used for prioritization or risk assessment activities in a Canadian regulatory context to date. Li et al. (2018) demonstrated the transport and fate of polychlorinated biphenyls (PCBs) from the indoor environment to rural environments, indicating that residence time of PCBs in the far field outlasts that of the near field and, therefore, human exposure to PCBs from foodweb pathways can be significant over time.

Figure 3. Conceptual local far-field model for human exposures to PCBs from Li et al. (2018).



L. Li et al. *Environment International 117 (2018) 57–68*

Fig. 1. Model representation of the technosphere, and the indoor, urban and rural environments of the Western Baltic drainage basin. The area (A) and height/depth/thickness (H) of each environmental compartment are also given. The indoor area is calculated based on the fraction (27.7%) of total indoor floor area in the Stockholm urban area (Cousins, 2012). The urban area is the sum of the reported areas of "urban agglomerations" (defined as areas with > 500,000 population) within the modeled region (Demographia, 2017); the rural area is calculated by subtracting the urban area from the total regional area [the default in CoZMo-POP (Wania et al., 2006)]. Arrows indicate mass exchanges among the three environments of different scale.

5.2 Temporal scale

There are 2 aspects to temporal scale that are relevant for to this topic. The first aspect involves dynamic (non-steady-state) release conditions. Section 4.3 discusses the influence of chemical persistence when episodic releases occur, noting that how often a chemical is released and its residence time affect the temporal and spatial scales of exposure and that this, in turn, can influence whether acute or chronic toxicity data are relevant to and used for the risk assessment. Within the context of the CMP, the GoC has traditionally not applied dynamic multimedia fate and exposure models to risk assessment. There are a few reasons for this approach, including the lack of ability to fully parameterize the model for dynamic emission conditions, lack of dynamic multimedia models available for the local scale (notable exception is ECORAME; Jung et al., 2014) and general model complexity. However, several regional- and continental-scale dynamic models are available (for example, BETR; MacLeod et al., 2001) and could potentially be adapted or adopted for GoC purposes in a nested framework, as discussed above. Episodic releases will have the greatest impact on local exposures as regional- and far-field exposures from more persistent chemicals often achieve a steady-state condition. The EUSES model, for example, assumes continuous steady state emissions unless knowledge of intermittent release is available, upon which acute exposure and toxicity assessments are conducted for the local scale to deal with such short-term pulse emissions. The use of dynamic models for GoC exposure assessment purposes remains a point for discussion under this topic meeting, noting that dynamic mixing-zone models may be fit-for-purpose at the local scale in some instances.

The second temporal aspect, also discussed in part in section 4.3, involves long-term exposures from the local to the far field where exposure concentrations gradually increase over time due to a long residence time of a chemical in the environment. The combination of persistence and bioaccumulation criteria were designed to qualitatively address this issue. As mentioned earlier, current CMP approaches represent a steady-state snapshot of chemical exposure that do not fluctuate over time, because they do not currently consider the residence time of a chemical in a medium (or the entire environment). Incorporating chemical persistence into exposure concentration estimations will permit a temporal (and spatial) assessment of exposure, and may allow, for example, the evaluation of vulnerable regions (remote or regional) and verification of the effectiveness of risk-management measures.

5.3 Summary and reading

Assessing the potential exposure from chemicals released to the environment over various spatial and temporal scales on a routine basis would require the investigation of chemical fate and persistence as well as the emission pattern. Ultimately, if a “new approach” to environmental exposure assessment that integrates these factors were to be implemented in the context of the CMP, the development of a modelling approach that connects a series of environmental boxes, each containing its own model environment, would be required. Bonnell et al. (2018) suggest that 1 approach could involve the adaptation of multimedia models such as the Quantitative Water, Air, Sediment Interaction (QWASI) model developed for fate and behaviour of substances emitted to the Great Lakes (MacKay et al., 1983a) and then subsequently adapted for rivers (Mackay et al., 1983b) and for inorganic compounds (Mackay and Diamond, 1989). The QWASI model (or a similar model) could be further adapted to include a connected sequential series of river reaches to address local aquatic emission scenarios to rivers and drinking water sources. The QWASI could also be coupled with models such as RAIDAR for local- to regional-fate and foodweb interactions and a far-field model such as Globo-POP (Wania et al., 1995) or BETR-World (Toose et al., 2004; MacLeod et al., 2005). Regardless of the model(s) used, a nested fate and exposure model is desired such that the GoC can track the ultimate fate of organic chemicals in the environment and estimate more realistic exposures to ecological receptors and/or humans. As a result, the GoC will be able to modernize prioritization and risk assessment activities under the CMP.

Recommended reading:

- CHAPTER II EUSES (European Union System for the Evaluation of Substances). 2004. Background Document. Version 2.0. RIVM Report no. 601900005/2004. (National Institute for Public Health and the Environment), Bilthoven, The Netherlands. J. P. A. Lijzen and M. G. J. Rikken (eds.). Available at https://www.rivm.nl/bibliotheek/rapporten/601900005.pdf.

- Fantke, P., Ernstoff A. S, Huang, L., Csiszar, S. A., and Jolliet, O. 2016. Coupled near-field and far-field exposure assessment framework for chemicals in consumer products. *Environment International*, 94: 508-518. Available at https://www.sciencedirect.com/science/article/pii/S0160412016302288?via%3Dihub.

- Li, L., Arnot, J. A., Wania, F. 2018. Towards a systematic understanding of the dynamic fate of polychlorinated biphenyls in indoor, urban and rural environments. *Environment International*, 117: 57–68. Available at https://www.sciencedirect.com/science/article/pii/S0160412018304100?via%3Dihub.

6.0 Charge questions to the committee

The following 3 charge questions solicit feedback from the SC on (1) when exposures beyond the near-field (local) scale are relevant and should be considered in CMP chemical evaluations; (2) how the GoC might achieve a dynamic multi-scale fate and exposure approach; and (3) what might the advantages, disadvantages, and key uncertainties be for implementing such an approach. These charge questions were designed to solicit fit-for-purpose advice on new approach methodologies for this topic, considering current and future needs of the CMP, both for assessment and long-term chemicals management.

At the CMP SC's recommendation, the charge questions and subsequent discussion at the meeting will focus on ecological exposures.

Charge Question 1: Considering both prioritization and risk assessment activities, when is it appropriate to predict environmental concentrations beyond the local scale (that is, regional and far field)?

Key ideas to examine include:

- the temporal emission pattern (episodic releases vs. continuous)
- multiple dispersive release points
- sensitive remote environments
- persistence and mobility (residence time)

Charge Question 2: How can the GoC better integrate chemical fate at relevant spatial and temporal scales to reduce key uncertainties in predicted environmental concentrations for both prioritization and risk assessment activities?

Key ideas to examine include:

- the coupling of fate and emissions modelling (including wastewater treatment systems)
- dynamic-release scenarios
- the modification and/or integration of available models
- scalable multimedia modelling/conceptual approach to SimpleBox and human multi-scale models
- tiered approaches
- fit-for-purpose

Charge Question 3: What are the primary advantages/disadvantages and key uncertainties the GoC might expect from implementing dynamic and more spatially resolved exposure assessment approaches for CMP chemical evaluation? Describe ways to overcome the disadvantages.

Key ideas to examine include:

- the aggregation of exposure pathways
- the uncertainty and sensitivity of emission rate and pattern (mode of entry)
- data quality and availability
- practicality versus complexity
- the domain of applicability for the new approach (assumptions, limitations, boundaries)
- tiered approaches to exposure assessment
- model uncertainty

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Appendix 1: Example local-scale model parameterization

Environmental concentrations used in CMP assessments reflect exposure close to the point of discharge (that is, local exposure), typically involving a media dilution approach. The estimation of emission concentrations is based on either industrial or household (down-the-drain) release scenarios, or both. Site-specific information (for example, use quantity, types of on-site and off-site wastewater treatment) combined with generic assumptions (for example, emission factors from the OECD emission scenario documents) is extrapolated across Canada to characterize a range of potential exposure situations.

Local-Model Parameterization (water emission scenario example)

Many different parameters are required in exposure calculations.

1) Tonnage: Information on use quantity for existing substances normally obtained via responses to section 71 surveys conducted with industry (for example, the DSL Inventory Update). The information collected reflects the data for the specific year(s) of the survey(s) and, as such, provides only a snapshot in time from that given year. Data collected for different substances within a single assessment may also have been surveyed during different periods of time, resulting in challenges in interpretation of the total quantities reported. In order to address some of these data gaps and reduce uncertainty, other sources of information on tonnage are consulted, such as the Canadian Border Security Agency data (import volumes for different codes, per year). Other tonnage estimate approaches include the use of maximum-facility capacity to determine how much of a substance may be used by a facility.

   In order to gather knowledge on tonnage trends for existing substances information from other jurisdictions is also consulted [for example, Substances in Preparations In the Nordic countries (SPIN) database and Chemical Data Reporting from the U.S. EPA] and used qualitatively to assess potential tonnage changes in Canada. Information on substances contained in products, articles, and manufactured items is difficult to obtain. Importers do not necessarily have the knowledge on the composition of their products.

   Annual tonnage data for new substances is a required element to be supplied with the notification to the GoC under the *New Substances Notification Regulations*. The notifier will identify the anticipated quantity of the substance manufactured, imported into, or exported from Canada over the coming 12 months and the maximum annual quantity over the next three years. In addition, they will indicate the annual quantity for each type of use for the substance.

   In order to anticipate future volumes beyond the notifier's intended activities, historic volumes identified by other notifiers for the substance or similar substances may be consulted through internal databases. In addition, similar to the existing substances approach, information from other jurisdictions may also be consulted as required.

2) Emission factors and other industrial parameters: Information on emission factors is most commonly obtained from generic information sources such as OECD emission scenario documents. When monitoring data from industrial effluent are available, this

may also be used to determine Canadian-specific emission factors for given sites and extrapolated more broadly to a whole sector. On-site mitigation measures are also factored in when suitable information is available. A compilation of release estimation or measurements (for example, National Pollutant Release Inventory) may also be used to determine emission factors. Estimating emission factors resulting from the use of products and articles is addressed on a case by case basis, often qualitatively only. Other industrial parameters of relevance (for example, number of days of operations, on-site treatment) are determined either by using generic information sources [for example, Technical Guidance Document (TGD) tables] or based on information from industrial facilities (for example, via follow-ups or site visits).

3) Wastewater treatment: Fate and removal rate in wastewater is most commonly estimated using models such as SimpleTreat v3.0 and sewage treatment plant model STP-EX, but in some instances it is determined based on monitoring data or supporting scientific literature. Mass-balance models for fate in wastewater treatment systems (WWTSs) cover primary, secondary, and lagoon (STP-EX only) systems. The WWTS mass balance is predominantly used to derive the mass fraction discharged to surface waters as well as biosolids. When a high-mass fraction of chemical in biosolids is predicted, the model biosolids concentration is used in combination with application rate data to derive an annual input to agricultural soils. It is assumed that industrial facilities discharging to sewers do not have on-site wastewater treatment. When there is indication of on-site industrial treatment, the treatment is assumed to be primary treatment. Industrial facilities that discharge directly to the environment are typically assumed to have secondary or equivalent-level treatment.

4) Dilution and receiving water body flows: Dilution and receiving water body flows are required to determine concentration in aquatic media. Information on flows of effluent from WWTS are obtained from a variety of sources [for example, Effluent Regulatory Reporting Information System (ERRIS), municipal websites, provincial compilations] and flows of effluent from industry are obtained from industry directly, consultant reports, or other sources of information. Surface water flow rates are obtained from Canadian Hydrometric Data (HYDAT) when such data is available for a location. Distribution of dilution and flows for water bodies receiving effluent from industrial facilities or from a domestic WWTS associated with industrial facilities have been compiled for different industrial sectors. Flow rate percentiles (for example, 10th, 50th)

are extracted for the distributions to represent varying dilution conditions across Canada, as appropriate. A dilution factor of 10 is often used to account for exposure very close to point-source releases in cases where river dilution is exceptionally large (for example, St. Lawrence River).

Appendix 2: Basis for local predicted environmental concentration (PEC) calculations

1) Aquatic: Exposure resulting from point-source industrial releases is typically estimated using a simple equation linking quantity, release, and flow information. Exposure resulting from down-the-drain releases is estimated using a population-based (per-capita usage) probabilistic model. The model works using known distributions of input parameters for per-capita water use, dilution factor, and treatment level. Plumes or mixing zones are typically not considered in the determination of an aquatic PEC, and concentration is determined at the point of discharge (assuming instantaneous dilution). The receiving environment may be an actual water body receiving effluent (representative site specific) but may also be a generic flow determined from flow distributions (Appendix 1).

2) Soil: The concentration in soil is based on an approach from ECHA (originally European Union TGD) for biosolids application to agricultural lands. The scenario considers the quantity of the substance accumulated in soil via yearly applications over 10 consecutive years. Generic input parameters (for example, soil depth, application rate, and frequency) reflect Canadian conditions. Degradation may be factored in, although other loss mechanisms (volatilization, leaching, run-off) are not typically accounted for. Exposures to terrestrial biota resulting from biosolids application are estimated on a case-by-case basis, depending on the intrinsic properties of the chemical (persistence and bioaccumulation) and on the emission rate to soil. Tissue residue approaches and mass-balance models [such as the Biosolids-Amended Soil: Level IV (BASL4)] are used. Atmospheric input to soil are generally not considered.

3) Sediment: Sediment concentrations are estimated in bottom sediment based on the equilibrium partitioning between the water column and sediment. The total concentration in the overlying water column is assumed to consist of 2 phases (aqueous phase and suspended sediment) and is assumed to reach a partitioning equilibrium state between its 2 phases as well as with the underlying bottom sediment. The approach takes into consideration the concentration of the substance in dissolved water, the suspended solid concentration, and the partitioning between phases (water, organic carbon). It is applicable to neutral organic substances for which organic matter is the primary phase of sorption driven by hydrophobicity. The approach can be extended to ionizing substances to provide conservative estimates of concentrations in sediment if they are not completely ionized. The model is parameterized using default properties of suspended and bottom sediments.

4) Air: Exposure in air is typically determined for very volatile substances or for substances for which the main release pathway is air. Typically, industrial releases from point sources are considered. Air concentrations at the end generic industrial facility (fenceline values) are determined. Air concentrations are determined using third-party models such as AERSCREEN and SCREEN3 for screening cases and AERMOD for more complex situations or when deposition estimates are required. Atmospheric PECs are based on generic default stack parameters (size, exit velocity, etc.).

5) Predatory wildlife: Concentrations in predatory aquatic and terrestrial biota are typically derived using a bioenergetics total daily intake (TDI) exposure model and/or a tissue residue approach.