PETROLEUM TECHNOLOGY ALLIANCE CANADA

Standardized Approach to Risk Assessment Based on Residual Mass versus Numerical Endpoints

Advancing Sustainable Contaminated Site Management in Alberta

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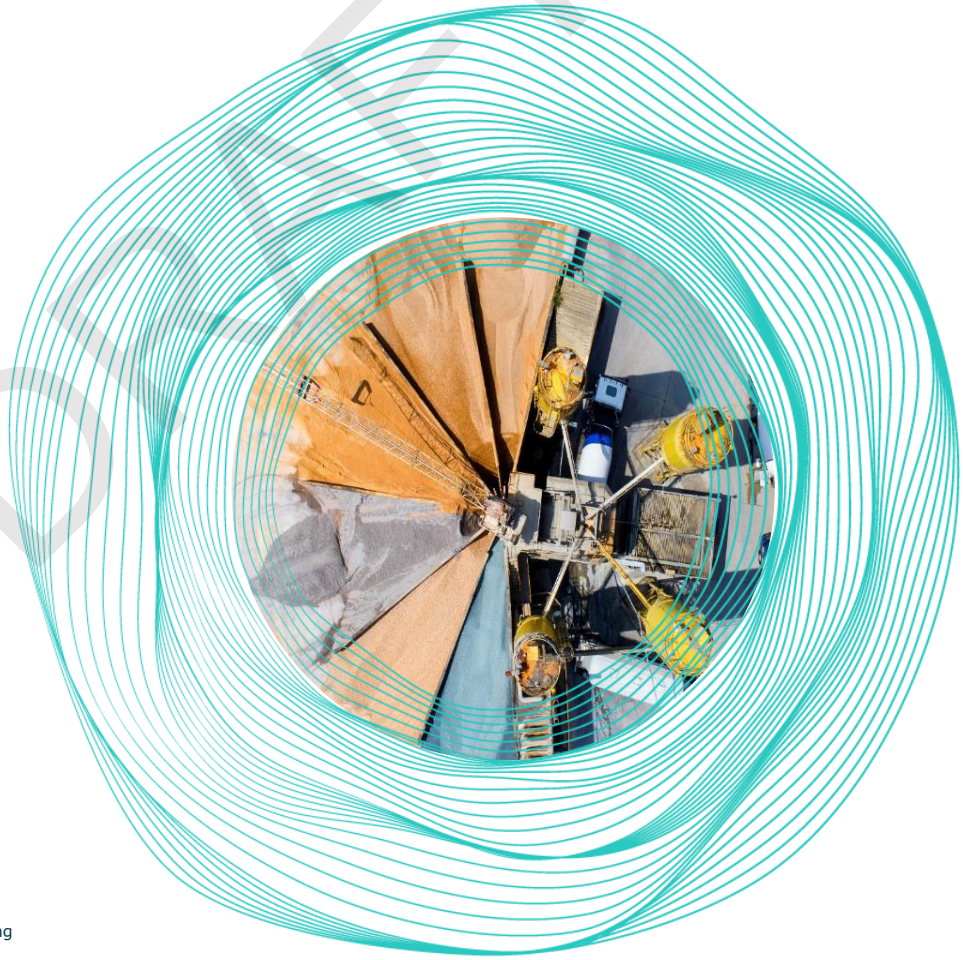

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Executive Summary

This report, prepared for the Petroleum Technology Alliance Canada (PTAC) by Worley Canada Services Ltd. operating as Worley Consulting (Worley), outlines risk assessment methods based on residual contaminant mass rather than traditional concentration-based endpoints. While published guidance in Alberta such as the use of fate and transport modelling, plume stability assessments, demonstrated natural attenuation processes, and weight of evidence and triad approaches in ecological risk assessment, current regulatory policy in Alberta prioritizes concentration-based guidelines as a measure of environmental effects. Relying solely on concentration-based guidelines overlooks factors that influence toxicity, such as the distribution of contaminant mass across different environmental matrices, source strength, and transport mechanisms that affect exposure over time. The mass-based approaches described herein offer a more comprehensive and realistic assessment of contaminant behaviour and potential impacts across varied environmental contexts.

Key risk assessment methods, described herein, that rely on residual contaminant mass rather than concentration-based endpoints include:

- total mass of contaminants;
- mass flux and discharge quantification;
- mass loading;
- mass transfer assessments;
- mass partitioning analysis; and
- mass balance modelling.

These tools provide insights into contaminant transport mechanisms, long-term exposure risks, and remediation effectiveness, enhancing the ability to prioritize and manage contaminated sites effectively. Case studies for select methods are presented demonstrating their applicability to contaminated sites practicality. The case studies presented consider a mass partitioning analysis of polychlorinated biphenyls (PCBs) in the Hudson River; a mass flux assessment of an industrial spill in southeast Alberta; and the development of an empirical mass balance model for the Lower Passaic River, part of the Diamond Alkali Superfund Site in Newark, New Jersey.

The report highlights how integrating these advanced approaches as risk assessment alternatives into Alberta's existing regulatory framework will improve risk assessment outcomes, lower unnecessary remediation costs, and strengthen environmental stewardship. Uncertainty around standardizing risk-based methods is also described herein. The report also presents a rough order of magnitude cost estimates for applying these methods to a standard oil and gas lease in Alberta and identifies the types of sites where they could be used.

Based on the findings of this review, it is recommended that expanded options for use of mass-based endpoints be incorporated as acceptable methodologies for use in risk assessments in

Alberta. This will effectively align Alberta's practices with international standards and guidance, fostering more effective remediation strategies, and supporting sustainable economic development.

1. Introduction

Petroleum Technology Alliance Canada (PTAC) retained Worley Canada Services Ltd. operating as Worley Consulting (Worley), to assess alternative risk assessment methods based on residual mass rather than concentration of a substance in the environment. The work presented herein focuses on evaluating effects based on total quantity (mass) of a contaminant rather than relying solely on concentrations of a contaminant compared to numerical endpoints, such as guidelines and/or screening levels.

Numerical endpoints provide an effective tool for rapidly screening large data sets. However, a parameter concentration above a guideline does not necessarily infer unacceptable risks to individual receptors as guidelines and screening levels are developed based on conservative assumptions and are meant to be broadly protective of a range of exposure scenarios. Comparison of concentration-based endpoints directly to guidelines or screening levels typically does not account for factors that modify exposure or toxicity. For example, a single concentration in an environmental media above guidelines is not representative of a widespread risk, as it ignores spatial variability and assumes receptor exposure is confined to that specific location.

A mass-based approach considers the total amount of contaminant (e.g. kilograms or grams) available to move through the environment or interact with receptors. This approach provides a more comprehensive understanding of the potential impact contamination may have on receptors over space and time. By focusing on overall mass, risk assessments can better account for cumulative effects, effects of long-term residual contaminants, and contaminant migration, which may not be apparent from concentration-based assessments alone. This is particularly useful in situations where contaminants are dispersed over large areas where their transport mechanisms can significantly influence risk, or where localized hotspots or areas with high residual concentrations require targeted assessment.

Numerous methods outlined in risk assessment guidance address mass-based approaches, depending on the type of receptor, and receiving environment under consideration. While Alberta policy and the current regulatory framework such as the use of fate and transport modelling, plume stability assessments, demonstrated natural attenuation processes, and weight of evidence and triad approaches in ecological risk assessment, it places limited emphasis on more advanced mass-based methods despite their broad applicability in contaminated sites risk assessment. As such, the assessment herein will explore the applicability of more advanced mass-based alternative methods to contaminated sites in Alberta and provide recommendations for integrating them into Alberta's regulatory framework to enhance risk assessment practices.

1.1 Goals and Objectives

The evaluation of alternative risk assessment methods for contaminated sites in Alberta has three key goals: 1) improve sustainable outcomes of remedial programs in Alberta; 2) reduce costs to

site closure[1]; and 3) enhance review efficiency within the Alberta regulatory system. Collectively, these improvements will create a more effective and sustainable contaminated site management framework for Alberta.

The objectives of the report, presented herein, are to:

- identify and evaluate methodologies that assess human health and ecological risk based on residual contaminant mass which are not currently incorporated into Alberta policy; and
- evaluate the applicability of these alternate risk assessment methods that apply mass-based endpoints for use on contaminated sites in Alberta.

1.2 Scope

The scope of this document addresses the objectives of identifying alternative methods for quantifying risks at contaminated sites in Alberta, moving beyond traditional concentration-based estimates. The report presents a comprehensive literature review that collates alternative mass-based risk assessment methods from various regulatory and technical sources, including federal, provincial and international jurisdictions (see Section 1.3.1 for more detail). The methods evaluated are not currently incorporated into Alberta's regulatory framework and include quantification of total mass of contaminants; mass partitioning analysis; mass flux and mass discharge quantification; mass transfer assessment; mass loading to sensitive receptors; and mass balance modelling. The review details the applicability of these methods to contaminated sites; their data requirements; their advantages and limitations; and a rough order-of-magnitude (ROM) cost estimate for implementation on a standard oil and gas lease. The review is supplemented by case studies where available. Uncertainties around standardizing these approaches are also documented. Additionally, the evaluation explores how these approaches can be integrated into broader, holistic frameworks currently recognized by Alberta such as fate and transport modelling, plume stability assessments, natural attenuation assessments, and weight of evidence and triad approaches, enhancing their applicability to comprehensive risk assessment.

1.3 Approach

This section provides an overview of the approach taken to completing the literature review, providing a cost comparison for implementation of different methods and the limitations associated with this review.

1.3.1 Literature Review and Key Sources

Key references use for the literature review included:

- Alberta Environment and Protected Areas (AEPA), Alberta Environment and Parks (AEP) and Alberta Energy Regulator (AER) policy and guideline documents;

[1] In Alberta site closure refers to the regulatory process of confirming a contaminated site has been sufficiently assessed and meets criteria such that risks to human health and the environment are negligible. Closure can occur through a Reclamation Certificate, which does not provide relief of liability; a Remediation Certificate, which provides relief of liability; or a Tier 2 Compliance Letter, which provides confirmation that Tier 2 Guidelines are acceptable in a case where remediation is not required, but does not provide liability relief.

- Other Canadian federal and provincial guidance documents;
- United States Environmental Protection Agency (USEPA) federal and regional guidance documents;
- Australian federal and regional guidance documents;
- Technical and Research Organizations:
  - Naval Facilities Engineering Command (NAVFAC);
  - Cooperative Research Centre for Contamination Assessment and Remediation of the Environment (CRCCARE);
  - Interstate Technology & Regulatory Council (ITRC); and
  - United States Geological Survey (USGS);
- Textbooks;
- Environmental Tools and Models; and
- Scientific Journals.

The literature review identified several mass-based risk assessment methods not currently incorporated into Alberta's regulatory framework, which are described herein. Sections 3 through 8 provide an overview of each method evaluated, including a description of its framework, the approach used to implement it, and practical applications of the methods. Case studies have been included to demonstrate the practical application of select methods in real-world scenarios (Appendices A through C).

Throughout the report, specific environmental media (e.g. soil, groundwater, surface water, etc.) are discussed in relation to the mass-based risk assessment methods. However, these examples may not cover the full range of media each method can assess. For a complete list of applicable media utilized by each method, refer to the dedicated "Media Considered" subsection within each chapter.

1.3.2 Development of Rough Order of Magnitude (ROM) Cost Estimates

ROM cost estimates for each method are provided to offer some practical perspective on method implementation. These estimates are based on a standard oil and gas lease in Alberta, typically an upstream site, such as a well pad, battery, or small processing facility, without unusually complicating factors (e.g. large spills, co-located industrial activity). The area of environmental concern (AEC) considered is a contaminant plume spanning approximately 50meters (m) in length and 20 m in width, groundwater depths less than 10 m, and 10–20 monitoring wells already in place to characterize site complexities. Emphasis is placed on cost-effective data collection methods that align with the goals of remediation planning, risk assessment, and maintaining regulatory compliance. Cost estimates are approximate and may vary depending on site-specific conditions, regional labor costs, mobilization times, accessibility, and the complexity of contamination at a site.

For purposes of providing ROM cost estimates for each method, the following assumptions have been included:

- The site is rated as moderately complex with hydrogeological conditions typical for Alberta.
- The site lacks unusual characteristics that would necessitate a more robust site assessment than standard protocols, including, but not limited to: fracture flow dominated contaminant transport; organic soils; unusually high permeability materials / preferential pathways; and/or discharge of contamination directly to stagnant water bodies and/or receiving environments, such as water supply wells.
- Only soil and groundwater are evaluated as part of the conceptual site model (CSM); soil vapour, surface water, porewater, and sediments are explicitly excluded from the CSM.
- A robust CSM has already been developed with comprehensive vertical and lateral delineation, adequate sampling resolution, and a clear depiction of contaminant sources and distribution, transport pathways, and potential exposure pathways. The existing site data from the CSM is available for use.
- Data needs presented herein are limited to those data that are in addition to the CSM.
- The site has up to twenty contaminants of potential concern (COPCs), drawn from petroleum hydrocarbons (PHCs), polycyclic aromatic hydrocarbons (PAHs), metals and trace elements, salinity parameters, and volatile organic compounds (VOCs).
- Regulatory reporting adheres to standard Alberta guidelines, including the Alberta Tier 1 and Tier 2 Soil and Groundwater Remediation Guidelines (AEPA 2024a; 2024b), Alberta Environmental Site Assessment (ESA) Standard (AEPA 2024c), Alberta Contaminated Sites Policy Framework (AEPA 2023), Supplemental Guidance on Site-Specific Risk Assessment *[SSRA]* in Alberta (AEP 2023), and AER requirements (e.g. Manual 021 [AER 2025] and assorted Directives). Submissions meet expectations outlined in these documents for data quality and plume delineation. Monitoring wells are installed for routine groundwater monitoring and available for use.
- The site is accessible by standard vehicles year-round, with no significant logistical challenges such as extreme weather delays, restricted access periods (e.g. spring breakup), or requirements for specialized equipment like helicopters.

1.3.3 Limitations

Below is a list of limitations that may be associated with the present document, which has been developed exclusively through a desktop literature review.

- **Potential Gaps in Available Literature** –The review is constrained by the quality, completeness, and relevance of available published sources. If key regulatory or technical documents lack detail, contain outdated information, or omit critical case studies, the analysis may be incomplete or biased.
- **Limitations in Literature Selection:** The document is generally focused on publicly available standards and guidance documents and the inclusion of non-public literature is limited.
- **Uncertainty in Cost Estimates:** Order-of-magnitude cost estimates are based on literature values rather than actual site implementation, which may lead to under or overestimation of costs dependent on site-specific conditions such as, but not limited to, location, accessibility, local terrain, contaminants, stratigraphy / geology, and other similar considerations.

- **Lack of Stakeholder Input:** The document was prepared with limited engagement with regulators, industry practitioners, and other stakeholders which may create limitations for applicability to some sites.
- **Limited Validation of Mass-Based Approaches in Site-Specific Risk Scenarios in Alberta:** Without testing the application of mass-based approaches on real sites in Alberta, the effectiveness and applicability of mass-based methods in risk quantification to sites in Alberta remains theoretical rather than demonstrated through direct implementation.
- **Limitations on Standardization of Mass-Based Endpoints:** Mass-based approaches in SSRA are inherently difficult to standardize due to the highly variable nature of contaminated sites in Alberta and the differing objectives and methodologies used to evaluate risk. While these approaches incorporate standardized requirements for data collection and interpretation, their applicability and value are ultimately governed by site-specific conditions. Within the current Alberta policy, mass-based approaches tend to be recognized as supplementary line of evidence for complex sites requiring an advanced SSRA rather than as broadly applicable decision-making tools. If Alberta were to incorporate a standard approach to mass-based endpoints more broadly into their policies, additional guidance would likely be needed to establish standardized processes, define limitations on applicability, clarify assessment objectives, and specify requirements for follow-up validation and long-term performance monitoring.
- **Static Snapshot of Knowledge:** The findings will reflect the state of knowledge at the time of the literature review, potentially missing emerging methods, technologies, or regulatory updates that occur after the study period.

2. Fundamental Concepts

Mass-based approaches emerge from the need to address the limitations of traditional contaminant assessment in complex settings. Understanding contaminant mass offers a more effective way to evaluate risks and the dynamics of contaminant plumes. This section introduces the core concepts behind mass-based techniques, linking their significance in addressing diverse contamination issues with the foundational principles that define their application and interrelationships.

2.1 Background

In Alberta, risk assessments completed for contaminated sites have traditionally relied upon numerical endpoints, such as regulatory guidelines and screening levels, to evaluate potential risks to human health and the environment (AEP 2023; AEPA 2023; 2024a; 2024b). While these benchmarks provide a standardized and efficient tool for initial evaluations, they often fail to address the complexities of contamination in diverse environmental contexts. This approach incorporates conservative assumptions to ensurethe values can be applied to most sites within a given land use category without conditions or restrictions, which often results in an overestimation of risks. Overestimating risks to receptors often to remedial efforts that are unnecessary to achieve the required risk reduction, leading to excessive costs, as well as environmental and social impacts.

The limitations of using generic numerical endpoints such as guidelines and screening levels underscores the need for alternative risk assessment methods that account for contaminant behaviour and interactions with environmental media and receptors. These alternative risk assessment methods provide for a more comprehensive and nuanced understanding of risk by focusing on residual contaminant mass, transport dynamics, variability, and cumulative impacts. For instance, mass flux/discharge quantification evaluates how contaminants move through environmental media, allowing for a better understanding of potential effects leading to more targeted and effective interventions. Triad approaches integrate real-time data collection and adaptive strategies to refine risk evaluations rather than relying solely on concentration data. Similarly, weight of evidence frameworks combine multiple lines of evidence to form balanced, science-driven conclusions.

Alternative risk assessment methods are particularly relevant in Alberta, where industrial activities have created a diverse array of contaminated sites that vary in size, complexity, and geographic distribution. Large facilities such as gas plants, refineries, mines, and chemical facilities are spread across the province, while smaller, more localized sites, including oil and gas leases, pipeline releases, compressor stations, substations, and gas stations, also contribute significantly to Alberta's contaminated sites portfolio. Given this variability, risk assessment methods that can effectively distinguish between discrete and widespread contamination are essential for protecting human health and the environment while optimizing remediation efforts and expenditure of fiscal resources. Implementing targeted risk assessment approaches will enhance the decision-making

process such that remediation efforts are proportionate to site-specific risks while supporting sustainable land management in Alberta.

Despite the broad applicability and advantages of utilizing mass-based endpoints in risk assessment, Alberta's regulatory framework has yet to fully integrate these advanced risk assessment methods. Existing Alberta policy (AEP 2023; AEPA 2023; 2024a; 2024b; 2024c; AER 2025) recognizes the applicability of some mass-based evaluations to quantify risks to receptors. These approaches include fate and transport modeling, plume stability assessments, natural attenuation assessments and use of mass-based lines of evidence as part of a weight of evidence approach to evaluate risk to ecological receptors. However, existing policy and guidance generally does not address the application of more advanced mass-based approaches to quantifying risks in SSRA. Incorporating these more advanced mass-based methods into regulatory policy could enhance the accuracy and efficiency of risk assessments, maximize sustainable outcomes, reduce costs for site operators, and streamline regulatory reviews. A more flexible and science-based framework would also allow Alberta to enhance environmental stewardship while supporting sustainable economic development.

2.2 Principles and Interdependencies

Mass-based approaches center on quantifying and analysing the behaviour of contaminant mass within environmental systems. This approach provides a structured method to track the presence and movement of contaminants across various media. These approaches hinge on measuring the total amount of contaminants—either contained within a specific zone or mobilized through a system—and evaluating how this mass interacts with its surroundings over time. Key principles include assessing the rate of contaminant flow through defined areas (mass flux), the transfer of contaminants between phases like soil, water, or air (mass transfer), and the distribution of contaminants across these phases based on their chemical properties (mass partitioning). Together, these elements offer a detailed picture of how contaminants persist, migrate, and transform at a site.

The application of mass-based approaches can be standalone or interconnected, depending on the objectives of the assessment. Individual methods, such as calculating total contaminant mass or analysing mass flux, allow for targeted insights into specific aspects like the extent of contamination or its migration patterns. However, many techniques build on these foundational tools. For instance, mass discharge integrates mass flux across a broader plane to quantify total contaminant movement, while mass loading accounts for the contaminant mass reaching receptors by incorporating empirical or modelled attenuation factors. Mass balance modelling ties these components together, using inputs like mass flux, mass transfer, and mass partitioning to verify mass conservation across the system. This interplay of mass-based approaches to risk assessment creates a versatile and cohesive framework for assessing contaminant pathways and dynamics across environmental compartments.

Table 2-1 summarizes the approaches outlined in this document, detailing their interdependencies and independent applications. Figure 2-1 provides a visual representation of how the different mass-based approaches are related. Sections 3 through 8 provide a more comprehensive review

of each referenced method, including how they can be integrated with or used to augment current mass-based methods allowed in Alberta (AEP 2023).

Table 2-1: Overview of Mass-based Assessment Approaches and Their Interdependencies

Approach	Definition	Interdependence	Independence
Total Mass of Contaminants	Represents the total contaminant mass within a defined source zone or environmental compartment.	Mass Flux, Mass Discharge, Mass Loading, Mass Balance	Can be independently estimated using concentration and volume data.
Mass Partitioning	Evaluates how contaminants are distributed among different environmental media (e.g. water, soil, air) based on partitioning coefficients (e.g. K_d, K_{oc}), helping to predict the final distribution after contaminant migration has occurred.	Mass Transfer, Mass Flux, Mass Balance	Can be independently assessed to understand contaminant behaviour across phases.
Mass Flux	Measures the rate at which a contaminant passes through a defined cross-sectional area per unit time (e.g. mg/m²/day).	Mass Discharge, Mass Loading, Mass Transfer, Mass Partitioning, Total Mass of Contaminants, Mass Balance	Can be used independently for localized plume assessment.
Mass Discharge	The total contaminant mass moving through a defined plane over time, integrating mass flux across the entire cross-section (e.g. g/day).	Mass Flux, Mass Balance	Cannot be determined independently as this method requires mass flux data.
Mass Transfer	Describes the movement of contaminants between different environmental phases (e.g. from soil to groundwater or from groundwater to air).	Mass Partitioning, Mass Flux, Mass Balance	Can be independently analysed for phase transitions but often requires mass partitioning data for accurate results.
Mass Loading	The total contaminant mass reaching a sensitive receptor over time, integrating mass flux and considering attenuation processes.	Mass Flux, Mass Balance	Cannot be evaluated independently as it depends on mass flux and attenuation data.
Mass Balance Modelling	A numerical or conceptual model accounting for inputs, outputs, and storage of contaminants within a system, to estimate total mass conservation.	Mass Flux, Mass Transfer, Mass Partitioning, Mass Loading, Mass Discharge, Total Mass of Contaminants	Cannot be evaluated independently as it requires data from multiple sources.

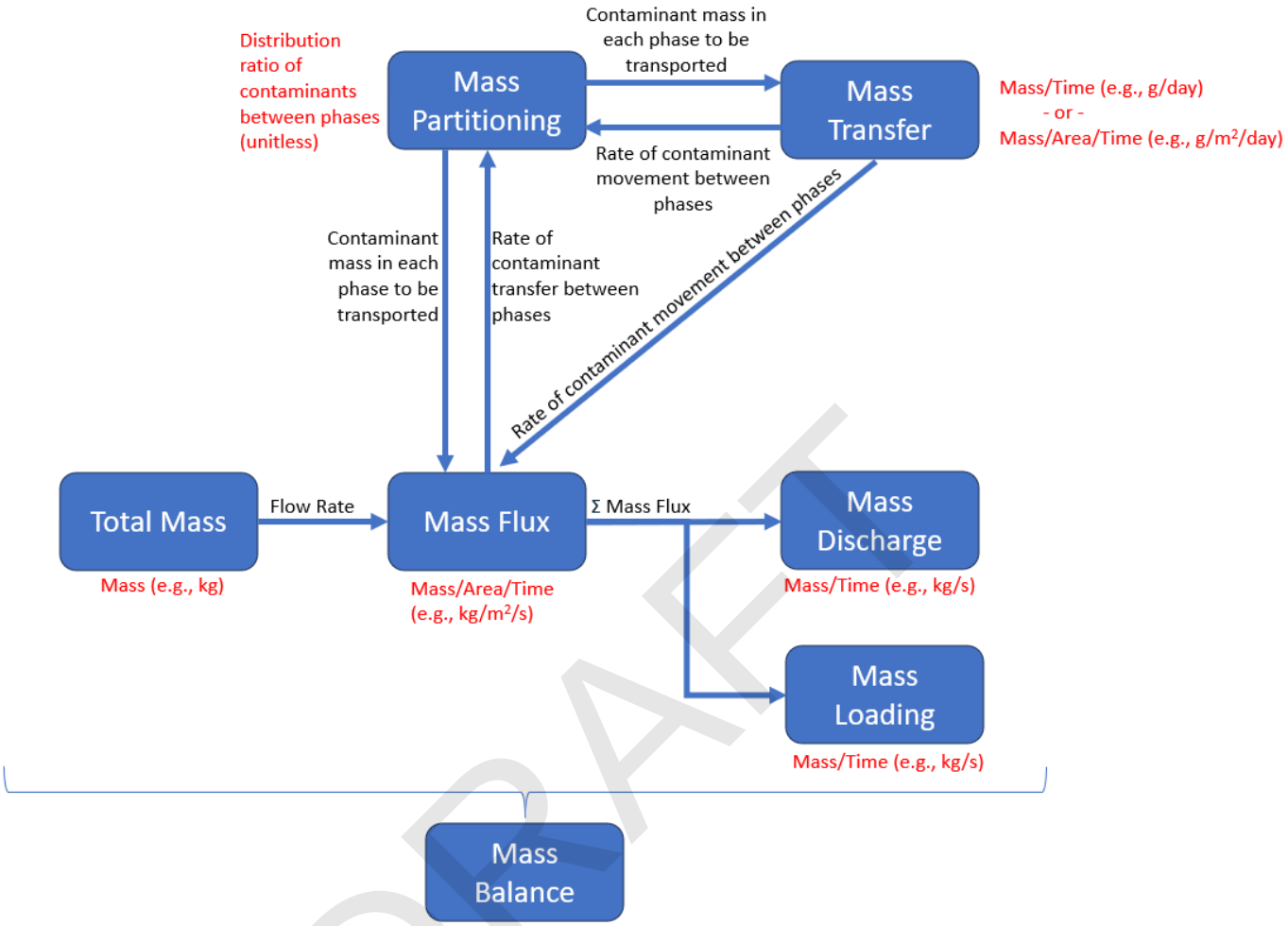

Figure 2-1: Relationship among mass-based approaches.
Red text indicates units. Red text: units of mass base approaches. Black text: describes relationships and processes between different mass based approaches.

3. Total Mass of Contaminants

3.1 Description

The total mass of contaminants at a contaminated site represents the cumulative amount of a contaminant present across environmental media. It accounts for contaminants in multiple phases (e.g. dissolved, sorbed, vapour, and non-aqueous phase liquids [NAPLs]) providing a comprehensive measure of the contaminant burden within the system. This approach integrates data from contaminant concentrations, phase partitioning behaviours, soil properties, and the physical dimensions of the contaminated zones. By summing contaminant mass across different compartments, the total mass estimate captures the overall contaminant load, offering insight into the potential for long-term persistence, future contaminant migration, and the potential effectiveness of remediation strategies.

Unlike concentration-based guideline analysis, which evaluates contaminant levels against regulatory thresholds at specific sampling points, total mass analysis provides a system-wide perspective on contamination. Concentration data alone may overlook contaminants stored in less mobile phases (e.g. sorbed onto soil particles or trapped in low-permeability zones) or dispersed across large volumes of soil or groundwater (USEPA 2019; Essaid et al. 2015). Moreover, the total mass of a concentrated source area can directly impact the adequacy of the inherent capacity of a system (e.g. an aquifer, surface water, sediments, or biota) to attenuate contaminant transport, which may be overlooked by a simple guideline analysis (Ford et al. 2008). As a result, concentration-based approaches might underestimate the long-term risk and persistence of contaminants, especially in heterogeneous subsurface environments. Total mass accounting addresses this limitation by integrating contaminant distribution across the site, allowing for better predictions of contaminant mobility, long-term exposure risks, and the potential for recontamination after remediation efforts.

3.2 Media Considered

Determining the total contaminant mass at a contaminated site typically involves evaluating multiple environmental media to capture the full extent of contamination across different phases and locations. These media include soil, groundwater, surface water, sediment, and vapour, each representing critical compartments where contaminants may exist in dissolved, sorbed, vapour, or NAPL phases.

- **Soil:** Soil encompasses both unsaturated (vadose zone) and saturated zones, where contaminants can adsorb to particles or persist as NAPLs, influenced by properties such as bulk density and organic carbon content.
- **Groundwater:** Groundwater is assessed as a key medium for dissolved-phase contaminants within aquifers, with its mass distribution influenced by hydraulic conductivity, porosity, aquifer properties and plume extent.
- **Surface Water:** Surface water, including streams, rivers, lakes, and wetlands, is included for dissolved contaminants, particularly in systems where porewater interactions occur.

- **Sediment:** Sediment in aquatic environments—such as riverbeds or lake bottoms—is evaluated for sorbed contaminants and NAPLs, reflecting depositional processes that concentrate contamination.
- **Soil Vapour:** Soil vapour in the vadose zone is considered for VOCs, which may partition from soil or groundwater, necessitating soil vapour measurements.

3.3 Approach

Estimating the total mass of contaminants at a contaminated site involves integrating data from multiple environmental media including soil, groundwater, surface water, sediment, and vapour to quantify the full extent of contamination across different phases and locations. The process begins with comprehensive site characterization, including full delineation of contaminant plumes, identification of source zones, and an assessment of contaminant phase distribution (e.g. dissolved, sorbed, vapour, and non-aqueous phase liquids [NAPL]). Sampling is conducted to collect concentration data across spatially representative points in each medium, providing adequate coverage to both high-concentration source areas and diffuse zones of contamination (Canadian Council of Ministers of the Environment [CCME] 2016). Properties of environmental media such as bulk density, porosity, organic carbon content, and moisture content are also measured, as they influence contaminant partitioning and mobility (CCME 2016; National Environment Protection Council [NEPC] 2011).

The total mass of contaminants is determined by quantifying contaminant mass in key compartments, including the dissolved phase in groundwater, porewater and surface water; the portion adsorbed to soil and sediment matrices; the vapour phase in the vadose zone; and the mass present as NAPLs within various environmental media (Naval Facilities Engineering Command [NAVFAC] 2018). The approach relies on specific calculations to estimate mass. The following points outline the specific methods used to assess the contaminant mass in each compartment:

- Dissolved Phase (Groundwater):
  - Measure concentrations in wells.
  - Estimate aquifer volume (thickness, porosity, plume extent).
  - Calculate mass: Concentration × Volume.
- Dissolved Phase (Porewater and Surface Water):
  - Evaluate levels in interstitial water and surface water bodies.
  - Determine volume of affected water.
  - Calculate mass: Concentration × Volume.
  - Note: this is critical in stagnant water bodies, such as Alberta wetlands, where contaminants accumulate.
- Adsorbed Phase (Soil and Sediment):
  - Measure concentrations in soil/sediment.
  - Estimate volume and bulk density.

- Apply the soil-water partition coefficient (K_d) for metals or the organic carbon-water partitioning coefficient (K_{oc}) multiplied by the fraction of organic carbon (f_{oc}) for organics in soil and sediment for partitioning.
- Calculate mass: Concentration × Volume × Bulk Density.

- Vapour Phase (Vadose Zone):
  - Measure VOC concentrations via soil gas sampling.
  - Estimate vadose zone volume and porosity.
  - Use Henry's Law constant to estimate partitioning.
  - Calculate mass: Concentration × Volume × Bulk Density.
- NAPL Phase:
  - Assess via core sampling or laser-induced fluorescence (LIF).
  - Estimate NAPL saturation and zone volume.
  - Calculate mass: Concentration or Saturation × Volume.

These mass estimates are often supported by geostatistical interpolation methods, such as kriging[2] or contouring, to model the spatial distribution of contaminants. Tools such as mass estimation spreadsheets or numerical models can be employed to integrate these parameters and calculate total contaminant mass in each compartment (NAVFAC 2018). The final total mass is the sum of calculated masses across media and phases, providing a site-wide estimate. This provides a comprehensive understanding of contaminant distribution across compartments and informs critical decisions related to plume stability, remediation strategies, and long-term site management. This approach may involve mass balance modelling (see Section 8) to reconcile discrepancies and create consistency across datasets. The final total mass estimate provides a holistic understanding of the site's contaminant burden, serving as a foundation for risk assessment, remedial design, and long-term monitoring plans.

3.4 Data Requirements

This section describes supplementary data that are required for total contaminant mass determination. These data are in addition to the data included within a detailed CSM as described in Section 1.3.2. For determining total contaminant mass, additional data focuses on quantifying mass across environmental media, rather than solely mapping distribution. As such, the following data are required:

- Phase Partitioning Coefficients: Information to evaluate contaminant distribution across dissolved, sorbed, vapour, and NAPL phases, using coefficients like K_d for metals (soil, groundwater, sediment), K_{oc} for organics (soil, sediment), Henry's Law constant for VOCs (groundwater, surface water to vapour), and the NAPL-water partition coefficient (K_{nw}) for NAPLs (soil, groundwater, surface water, sediment). Generally, these parameters can be collated from published literature; however, site-specific measurements and/or adjustments may reduce uncertainty in mass estimates.

[2] Kriging is a geostatistical interpolation technique that estimates unknown values at specific locations by calculating a weighted average of known data points, based on their spatial relationships, while also providing an uncertainty estimate.

- Physical Properties: Properties to adjust concentration data for mass estimates, including:
  - Soil: Bulk density, porosity, moisture content, f_{oc} (organic carbon fraction), grain size distribution.
  - Groundwater: Aquifer porosity, bulk density of aquifer matrix, temperature, moisture content of saturated zone (e.g. near water table).
  - Surface Water: Porewater saturation in associated saturated zones, temperature, flow rate and variability (if dynamic).
  - Sediment: Bulk density, porosity, moisture content, f_{oc}, grain size distribution.
  - Vapour: Vadose zone porosity, soil moisture content, temperature (which affects vapour pressure).
- Volume Estimates: Volumetric data to quantify contaminated media for mass calculations, including vadose zone thickness, aquifer plume volume (groundwater), surface water body dimensions (e.g. lake or wetland), sediment layer thickness and extent, and NAPL saturation zones.
- NAPL-Specific Data: For sites with NAPLs in soil, groundwater, or sediment, data from core sampling, LIF, or saturation estimates to quantify NAPL mass (e.g. core samples for soil, fluorescence for groundwater containing dense non-aqueous phase liquid [DNAPL]).
- Vapour Sampling: Soil gas concentration data (e.g. VOC levels) in the vadose zone above soil and groundwater, collected via targeted sampling.
- Porewater Sampling: Porewater concentrations in saturated zones beneath water bodies (e.g. wetlands, lakes), especially in stagnant Alberta systems where contaminants accumulate, paired with volume estimates.

3.5 Application

Table 3-1 table outlines key applications of total contaminant mass, describing their purpose, relevance, and practical uses in contaminated site assessment and management. Table 3-2 and Table 3-3 outlines site types where determining total contaminant mass is either beneficial or not required.

Table 3-1: Applications of Estimating Total Mass of Contaminants at a Contaminated Site Management

Application	Description	Key Uses
Site Characterization	Quantifies the total contaminant burden across different media (e.g. soil, sediment, water, vapour).	• Understand contaminant distribution across environmental compartments. • Identify high-mass contaminant zones (e.g. source areas). • Support CSM development.
Risk Assessment	Evaluates the potential risk based on the total contaminant mass present.	• Estimate long-term exposure risks. • Assess potential for contaminant migration and plume expansion. • Prioritize areas for remediation.

Application	Description	Key Uses
Remediation Planning	Informs the selection and optimization of remediation strategies based on total contaminant mass.	• Design effective remediation technologies (e.g. pump-and-treat, in-situ chemical oxidation). • Determine required treatment scale and duration. • Predict remediation outcomes.
Mass Flux and Discharge Analysis	Supports the calculation of contaminant transport rates through environmental media.	• Estimate contaminant migration rates across boundaries, such as interfaces between soil layers, aquifer edges, or designated cross-sections like a site perimeter or control plane, where contaminant movement is tracked. • Evaluate effectiveness of risk management measures. • Support regulatory compliance reporting by quantifying contaminant migration rates and total loads across boundaries like site perimeters or aquifers, assessing risks to receptors, evaluating remediation success, confirming plume stability, prioritizing high-risk areas, and providing precise data for mandated metrics like water quality standards.
Performance Monitoring	Tracks changes in total contaminant mass over time during remediation or natural attenuation.	• Measure remediation progress and effectiveness. • Verify achievement of remediation goals. • Identify residual contaminant mass hotspots.
Long-Term Site Management	Guides decisions for ongoing site management and monitoring programs.	• Plan long-term monitoring strategies. • Evaluate the need for additional remediation efforts. • Provides opportunities to implement sustainable contaminant management by contributing to a holistic CSM that balances environmental, societal, and economic factors to protect human health and the environment while minimizing harm (e.g. greenhouse gas emissions) and maximizing benefits (e.g. local economic growth) without compromising quality, cost, schedule, or productivity (Sustainable Remediation Forum [SURF] 2011).

Table 3-2: Relevant Sites for Determining Total Contaminant Mass

Type of Site	Reason	Limitations
Relevant Sites		
Hydrocarbon-contaminated sites (e.g. benzene, toluene, ethylbenzene, and xylenes [BTEX], petroleum hydrocarbon [PHCs], polycyclic aromatic hydrocarbon [PAHs]).	Total mass helps assess risks and develop remediation strategies.	Typically, does not account for attenuation of hydrocarbons or complex subsurface variability.
Sites with salt and brine contamination from produced water spills.	Useful for salinity management and assessing risks to soil, vegetation, and freshwater aquatic life (FWAL).	May overestimate risk in areas with natural dilution processes or fail to address risks associated with localized hotspots.
Sites with sulphur from abandoned or active mines, refineries or chemical plants, and areas with sour gas (H_2S) or sour-heavy crude oil spill.	Captures the full scope of contamination across media (e.g. sulphide in soil turning into sulphate in water or H_2S in air), ensures regulatory compliance, prioritizes risks, informs long-term management by addressing sulphur's persistence and reactivity, and accounts for complex pathways involving multiple forms, avoiding underestimation of exposure risks.	May not account for dynamic chemical transformations (e.g. sulphide to sulphate) or varying bioavailability influenced by site-specific conditions.
Sites with metal contamination due to equipment corrosion or catalyst releases (e.g. arsenic, lead, mercury).	Informs leaching potential from soils and helps identify risk management required.	May not considered potential metal speciation that can affect bioavailability and contaminant mobility.
Chemical additive contamination at midstream sites (e.g. glycols, amines).	Supports predictions of migration and breakdown pathways.	Limited accuracy if transformation products are not fully characterized.
Sites with persistent pollutants (e.g. sterilant, polychlorinated biphenyls [PCBs], and per- and polyfluoroalkyl substances [PFAS])	Reveals the full extent of the persistent pollutants long-lasting presence across environmental media, guiding effective cleanup and risk management.	Complex interactions with biota or variable degradation rates may complicate mass estimates.
Naturally occurring radioactive materials (NORMs) contamination from produced water or equipment scale deposits.	Aids in evaluating long-term risks to human health and environment.	Difficult to quantify low-level radiation contributions to total mass accurately.

Table 3-3: Unsuitable Sites for Determining Total Contaminant Mass

Type of Site	Reason
Small-scale or localized contamination (e.g. minor fuel spills).	Total mass determination may be unnecessary for minor impacts, particularly if the release occurred recently.
Sites with rapidly degrading contaminants (e.g. ethanol, methanol, phenol).	The total mass will overestimate risks due to degradation processes.
Diffuse or non-point source contamination (e.g. agricultural runoff, atmospheric deposition, impacted fill materials spread across a wide area).	Impractical or non-actionable for widespread contamination.

Type of Site	Reason
Sites with transient contamination (e.g. stormwater runoff).	Focus is on source control rather than quantifying residual contaminant mass.
Pathway-specific risk assessments (e.g. vapour intrusion, surface water impacts).	Concentration or pathway-based assessment is sufficient. Risks can be limited to a single media and concentration-based data support that risks are negligible in other media.
Sites with bound or immobile contaminants (e.g. asbestos, weathered hydrocarbons).	Rather than total contaminant mass, risk assessment relies on exposure pathways, containment concentrations and bioavailability.

3.6 Relationship to Alberta Policy

3.6.1 Current Status

The use of the total mass of contaminants as a decision-making tool in contaminated sites investigation, remediation and risk assessment is currently recognized within current Alberta policy as summarized below.

- Current AEPA and AER policy requires that full delineation of contamination in environmental media to Tier 1 guidelines or Tier 2 guidelines developed with pathway exclusion is completed for each site (AEP 2023; AEPA 2023; 2024a; 2024b; 2024c). This requirement does not explicitly require quantification of total mass but provides the needed data to quantify total mass and allows for total mass to be utilized to support CSM development and identification of source area (AEPA 2024c).
- While not explicitly documented within Alberta written policy and guidance documents, total mass has precedent of being an acceptable input in remedial options analysis (ROAs) and remedial action plans (RAPs) including to monitor remedial performance, assess NAPL plume stability, and monitor natural source zone depletion (NSZD) and natural attenuation processes. NAPL plume stability and natural attenuation assessments are documented as acceptable lines of evidence to support risk assessment and long-term risk management (AEP 2017; 2023).
- Total mass calculations are an acceptable line of evidence used to inform minimal exceedance assessments that are accepted by AER for low volume / concentration / mass contamination.
- While not explicitly documented within Alberta written policy and guidance documents, total mass has precedent of being an acceptable input in complex fate and transport modelling, particularly to establish boundary conditions for the model and support model calibration. Complex fate and transport models are documented as an acceptable line of evidence to support risk assessment and long-term risk management (AEP 2023).

3.6.2 Gaps in Alberta Policy and Opportunities for Improvement

There are gaps in Alberta's written policy and guidance about how to calculate total contaminant mass, which methods / guidance documents AEPA and AER consider acceptable, limitations on the applicability of total mass calculations, and what input parameters are acceptable. To address these gaps, it would be beneficial to provide formal written policy and/or guidance that describes:

- When AEPA / AER consider total mass to be an acceptable metric to describe contamination within a CSM;
- What site-specific conditions preclude the calculation of total mass to describe contamination within a CSM;

- What specific methods/guidance AEPA / AER considers acceptable when calculating total mass;
- What input parameters are acceptable including, as appropriate:
  - use of default parameters;
  - when site-specific data must be collected;
  - how to approach situations where site-specific information is unavailable and cannot be practically collected/verified; and
- When total mass can or cannot be used as a performance metric.

Providing written policy and/or guidance on the methods and key assumptions that are acceptable to AEPA and AER for estimating total mass would provide consistency in these evaluations, limit rework and minimize potential for both submission returns and supplemental information requests (SIR).

3.7 Costing

The table below presents an estimated cost breakdown for a simplified total contaminant mass calculation at a standard oil and gas lease in Alberta, focusing only on supplemental data collection beyond a comprehensive CSM limited to soil and groundwater. The cost estimates are derived from Section 0 (Data Requirements) and aligned with the assumptions in Section 1.3.1, excluding simulation predictions or complex modeling.

Table 3-4: Estimated Cost for Determining Total Contaminant Mass at a Standard Oil and Gas Lease

Task	Description	Cost Estimate
Project Planning and Data Review	Review existing CSM (soil/GW data from 10–20 wells), plan 10 soil samples, 5 NAPL boreholes, and geophysical survey locations; coordinate logistics (lab, equipment).	$2,250 - $3,000
Phase Partitioning Coefficients	Collect data for Kd (metals) and Koc × foc (organics) in soil and groundwater via lab analysis of existing soil samples (5 samples) and groundwater from 10 pre-installed wells; literature values used for Henry's Law and Knw.	$2,500 - $3,000
Soil Physical Properties	Measure bulk density, porosity, moisture content, and foc from 5 additional soil samples in areas of uncertainty (e.g. plume edges); assumes existing CSM data covers basic delineation.	$1,500 - $2,000
Grain Size Distribution	Conduct sieve analysis for grain size distribution on 5 soil samples to refine partitioning and mass estimates.	$250 - $500
Analyse Additional Soil and Groundwater Samples	Analyse additional 5 soil and 5 groundwater samples for 20 COPCs (PHCs, PAHs, metals, salinity, VOCs) beyond CSM baseline to refine total contaminant mass estimation; includes analysis of Kd for new soil samples.	$1,500 - $2,000
Field Labor and Equipment	Deploy field crew (2 technicians, 1 days) for sampling, LIF, and geophysical survey; equipment rental (e.g. LIF tool, coring rig) and vehicle access included, assuming year-round standard vehicle access.	$5,000 - $7,000
Data Compilation and Reporting	Compile supplemental data, calculate total mass (concentration × volume × adjustments), and prepare a summary report.	$5,000 - $7,000
Project Management	Oversee field activities, lab submissions, data compilation, and reporting; includes scheduling, quality assurance and quality control (QA/QC), and client/regulatory communication.	$3,000 - $4,500

Task	Description	Cost Estimate
Total Estimated Cost		**$21,000 – $29,000**

These estimates are approximate and can vary based on site-specific conditions, regional labor rates, and the complexity of the contamination. Costs will be reduced if data are collected concurrently with CSM development and/or execution of other field programs.

3.8 Summary

Use of total mass to quantify risk provides a relatively low-cost option that can be broadly applied to contaminant plumes on a range of sites. Data requirements are similar to those of typical site characterization and therefore this approach can be broadly applied for risk assessment, risk management and remedial planning with limited additional costs. This method also serves as a foundation for integrating additional mass-based techniques when more detailed analysis is warranted.

4. Mass Partitioning Analysis

4.1 Description

Mass partitioning analysis is used in contaminated site management and remediation to understand the distribution, behaviour, and fate of contaminants, as mass distribution in a multiphase system is determined by partitioning processes (CCME 2016; USEPA 2021a). Mass partitioning evaluates how contaminants are distributed between different environmental media (e.g. soil, groundwater, air) and phases (e.g. absorbed to particulates, free phase [e.g. NAPL], colloidal, and dissolved) at equilibrium, helping to predict the final distribution of contaminants after movement has occurred (Vignati et al. 2009). Understanding this distribution is crucial for predicting how substances behave in different environments, which has implications for pollution control, site management and remediation.

At contaminated sites, contaminants often exist in multiple phases, interacting with soil particles, water, and air in complex ways. For example, hydrocarbons from petroleum spills can partition into water, soil, and air depending on their affinity for organic carbon, solubility, and volatility. Mass partitioning analysis quantifies these interactions, enabling the prediction of contaminant transport and potential future exposure pathways, such as inhalation of vapours migrating to indoor air or ingestion of groundwater as plumes expand over time. By evaluating how contaminants distribute themselves among the sorbed, dissolved, vapour, and residual phases, practitioners can determine which pathways pose a risk to human and ecological receptors.

The primary factors influencing mass partitioning include contaminant-specific characteristics such as solubility, vapour pressure, and K_{oc} (Wania and Mackay 1999; Vignati et al. 2009; USEPA 2021a), as well as site-specific parameters like soil type, organic carbon content, moisture levels, and temperature (Bierman et al. 1992; Vignati et al. 2009; USEPA 2021a). However, relying on generic or default partition coefficient values from the literature can lead to significant errors when predicting contaminant migration or evaluating site-remediation options. For this reason, the USEPA (1999) emphasizes the importance of using partition coefficient values measured under site-specific conditions for accurate calculations. For example, site-specific conditions such as organic carbon content and contaminant properties influence partitioning behaviour. Hydrophobic organic contaminants (e.g. PCBs) are more likely to sorb onto soil organic matter, while volatile organic compounds (e.g. benzene or toluene) may partition more readily into soil vapour. Understanding these interactions helps refine risk assessments and prioritize remediation efforts.

Mass partitioning analysis is often performed using mathematical models that incorporate partitioning coefficients, site-specific data, and environmental parameters. Equilibrium partitioning models assume steady-state contaminant distribution across phases and use partition coefficients to estimate concentrations in each phase under chemical equilibrium (Bloch et al. 2022). Kinetic models may also be applied to simulate temporal changes in contaminant distribution. These models use differential equations, parameterized with site-specific rate constants where available; generic half-lives from literature may be available when site data are limited although Alberta-specific policy currently limits the use of published half-lives unless they are explicitly documented

in the Alberta Tier 1 Soil and Groundwater Remediation Guidelines (AEPA 2023; AEPA 2024a). Use of kinetic models allows for predictions of how chemicals migrate over time within a system (Bloch et al. 2022). Both types of models are supported by empirical data obtained from site investigations, such as soil and groundwater sampling, soil vapour surveys, and geochemical analysis.

Unlike concentration-based guidelines, which assess contaminants in isolation within a single phase, mass partitioning considers processes such as sorption, volatilization, and dissolution, offering a more accurate representation of contaminant fate, transport, and long-term risk (CCME 2016). This approach enables development and implementation of targeted remediation strategies, prioritizes critical exposure pathways, and supports sustainable site management decisions by allocating resources where they can effectively reduce risks.

4.2 Media Considered

Mass partitioning analysis assesses the distribution of contaminants across various environmental media at a contaminated site. Typically, the environmental media considered include soil, groundwater, surface water, sediment, soil vapour, and air, as these are the primary compartments where contaminants partition and influence fate and transport (CCME 2016; USEPA 2021b). Below is an evaluation of each medium's role in contaminant partitioning and behaviour.

- **Soil:** Soil is evaluated for contaminants sorbed to particles, present as free phases (e.g. NAPLs), or in residual forms. The partitioning behaviour is governed by interactions with organic carbon, clay content, and soil structure, which influence adsorption, desorption, and degradation processes. Variations in soil texture and water content further govern the diffusive and advective mobility of contaminants, as well as their bioavailability (CCME 2016).
- **Groundwater:** Groundwater is analysed for dissolved contaminants and colloidal fractions that facilitate subsurface migration and plume expansion. Partitioning into groundwater depends on solubility, hydrophobicity of a substance, physico-chemical properties of contaminants and the aquifer, and interactions with aquifer materials like organic matter or minerals. Processes such as advection, dispersion, and biodegradation affect contaminants transport to downgradient receptors and drinking water sources (CCME 2016).
- **Surface Water:** Surface water is included when contaminants enter receiving waterbodies such as streams, rivers, lakes, or wetlands, often via runoff, groundwater discharge, or direct release. Partitioning is influenced by physico-chemical properties of contaminants and water chemistry (e.g. pH, dissolved organic carbon, hardness, oxidation – reduction [redox] potential [ORP]), which affects solubility and speciation of contaminants. Surface water is inherent to evaluating aquatic exposure pathways, with potential for dilution, volatilization and sediment deposition altering contaminant fate (Vignati et al. 2009; CCME 2016).
- **Sediment:** Sediment is a key medium in aquatic environments, where contaminants may sorb to organic matter or mineral surfaces, settle from the water column, or persist as residual phases. Partitioning depends on sediment composition, grain size, and redox conditions, which control bioavailability and toxicity to benthic organisms. Sediment acts as both a sink and a source of contaminants, influencing long-term ecological risks (Vignati et al. 2009; CCME 2016).
- **Soil Vapour:** Soil vapour is evaluated for volatile and semi-volatile contaminants that partition into the gaseous phase within the unsaturated (vadose) zone of the subsurface. This medium

is essential for assessing how contaminants volatilize from soil or groundwater and move through soil pores, posing risks such as vapour intrusion into buildings. The partitioning into soil vapour is influenced by factors such as the contaminants vapour pressure, soil moisture content, organic carbon content, and temperature (CCME 2016; USEPA 2021b).

- **Air:** Air is assessed for volatile contaminants partitioning into the vapour phase from various terrestrial and aquatic sources, including soil surfaces, water bodies, or free-phase liquids. This medium focuses on how these contaminants, once released, behave in the atmosphere, driven by vapour pressure, temperature, and air exchange rates, leading to processes like atmospheric dispersion or deposition. Analysis of air is vital for understanding inhalation risks in outdoor settings and broader environmental exposure pathways (USEPA 2021b).
- **Biological Tissue:** In some cases, biological tissues (e.g. plants, fish, or other organisms) are considered when bioaccumulation studies quantify contaminants uptake from soil, water, or sediment. Partitioning into biota depends on factors like lipid content, metabolism, and trophic level, linking environmental concentrations to ecological and human health risks. This medium integrates exposure across other compartments, reflecting food chain transfer and biomagnification (USEPA 2000b).

4.3 Approach

Determining mass partitioning at a contaminated site combines field sampling, laboratory testing, literature review, and modelling to characterize contaminant distribution across environmental phases. The process typically begins with site characterization and sampling, where representative soil, water, sediment, air and tissue samples are collected, and key environmental parameters such as temperature, pH, organic carbon content, and redox conditions are measured. Laboratory testing, including sorption/desorption, biodegradation and transformation assessments, bioaccumulation studies and quantification of partitioning coefficients can provide data on how contaminants interact with various environmental media. These coefficients, in turn, inform contaminant distribution and mobility across different phases. Literature review can also be used to supplement site-specific data for well-studied contaminants. Modelling techniques are then used to integrate these data to predict contaminant behaviour and assess risks to the environment and human health. The following summarizes the methods and principles used to define mass partitioning at a contaminated site. These techniques can be used independently or in combination with other analyses to refine mass partitioning estimates.

Partitioning Coefficients

A partitioning coefficient quantifies the distribution of a contaminant between two different phases (e.g. organic carbon and soil/sediment or biota and an environmental medium) at equilibrium, providing a key metric for understanding mass partitioning. Partitioning coefficients (e.g. K_d, K_{ow}, K_{aw}) are determined in the laboratory using batch equilibrium or column leaching tests to quantify contaminant distribution across phases (USEPA 1999), with Canadian testing typically conducted by academic researchers using standardized methods, such as Organisation for Economic Co-operation and Development (OECD) protocols, rather than accredited commercial facilities. Alternatively, partitioning coefficients can be sourced from literature reviews and established databases when experimental data are unavailable to supplement site-specific findings. Mathematically, a partitioning coefficient represents the ratio of a contaminant concentration in

two phases at equilibrium (Schlosser et al. 2010). Thus, the partition coefficient, *K*, can be calculated using the formula:

$$K = \frac{C1}{C2} \qquad \textbf{Equation 4-1}$$

where:

C1 is the concentration in phase one (e.g. water) and *C2* is the concentration in phase two (e.g. soil). Three-phase partition models extend this concept by incorporating an additional phase, to account for partitioning across water (dissolved phase), soil (sorbent phase), and air (vapour phases) simultaneously, providing a more comprehensive representation of contaminant behaviour in the environment (Bierman et al. 1992).

Partitioning coefficients are classified based on the environmental media they describe, with each coefficient providing a quantitative measure of contaminant distribution and behaviour across soil, sediment, water, vapour/air or biota under equilibrium conditions.

- The soil-water partitioning coefficient (K_d) represents a contaminant's sorption to soil or sediment, including organic and inorganic components, relative to its concentration in water. K_d varies with soil composition and is highly influenced by organic carbon content for organic contaminants like petroleum hydrocarbons and PAHs, making comparisons across different soils inconsistent.
- The organic carbon-water partitioning coefficient (K_{oc}) normalizes sorption to the organic carbon fraction (f_{oc}), providing a standardized measure of a contaminant's affinity for organic matter. Unlike K_d, K_{oc} allows for direct comparisons across different soils and sediments, making it useful for predicting organic contaminant behaviour (USEPA 1999).
- The octanol-water partitioning coefficient (K_{ow}) indicates a contaminant's tendency to accumulate in organic materials, which is important for evaluating its potential for bioaccumulation in organisms (USEPA 1999).
- The air-water partitioning coefficient (K_{aw}) and Henry's Law Constant (H') describe how volatile compounds distribute between water and air, with H' specifically representing the ratio of a gas' concentration in air to its concentration in water (Sarraute et al. 2004).
- The soil-air partitioning coefficient (K_{sa}) helps evaluate the potential for vapour intrusion from contaminated soil into buildings or the atmosphere (Ahn et al. 2020). While these examples illustrate key partitioning coefficients, they represent only a subset of the many coefficients available, each named to reflect the specific relationships they quantify between environmental media.
- Media-tissue partitioning coefficients, such as the bioconcentration factor (BCF), bioaccumulation factor (BAF), and biota-sediment accumulation factor (BSAF), quantify the distribution of contaminants from environmental media (e.g. water, sediment) to biological tissues, providing insights into ecological and human health risks from contaminant uptake in organisms (USEPA 2000b; Government of Canada 2013).

Sorption and Desorption Testing

Sorption and desorption testing is conducted to evaluate how contaminants bind to soil particles (sorption) and how they can be released back into the environment (desorption) (CCME 2016; Kato 2021). These processes are influenced by factors such as soil composition, organic matter content, and contaminant properties, and are required for understanding the mobility and persistence of contaminants in soil and groundwater (CCME 2016). Testing involves equilibrating soil or sediment samples with contaminant solutions at varying concentrations under controlled temperature, pH, and agitation conditions, followed by phase separation and contaminant analysis to quantify sorption onto the solid phase (OECD 2000; Kato 2021). Desorption is then assessed by replacing the contaminant solution with a clean solvent or water, re-equilibrating, and measuring the contaminant released back into the liquid phase (OECD 2000; Kato 2021). The results of these tests help generate sorption and desorption isotherms, which describe how contaminants distribute between the solid (e.g. soil or sediment) and liquid (e.g. water) phases (OECD 2000; Bleam 2017). These isotherms are used to determine partitioning coefficients, such as K_{oc} (organic carbon to water partition coefficient) if f_{oc} is quantified or Kd (soil-water partition coefficient), which quantify the contaminant's distribution and help predict its mobility, retention, and potential for remobilization in the environment (OECD 2000; Bleam 2017).

Biodegradation and Transformation Assessments

Biodegradation and transformation assessments evaluate how contaminants change in concentration, chemical structure, and distribution across environmental phases (e.g. soil, sediment, water, air) due to biological or chemical processes (CCME 2016). These assessments track mass partitioning by monitoring the concentration of the contaminant and its breakdown products across different phases over time (King et al. 1999). Analytical methods such as gas chromatography and mass spectrometry are commonly used to quantify contaminant concentrations and their transformation products (USEPA 2008a). Additionally, compound specific isotope analysis (CSIA) can define where biodegradation and transformation processes are occurring by analysing isotopic fractionation of contaminants and their transformation products (USEPA 2008a). CSIA typically measures the stable isotope ratios of carbon, hydrogen, oxygen, nitrogen, sulphur and/or chlorine in individual volatile and semi-volatile compounds extracted from complex environmental mixtures. This method distinguishes between biotic and abiotic processes, by analysing changes in isotopic ratios (expressed in units of per mil), providing accurate information on contaminant breakdown and redistribution across environmental phases (USEPA 2008a). These advanced methods enhance the ability to evaluate contaminant fate and inform remediation strategies effectively (USEPA 2008a).

Bioaccumulation Studies

Bioaccumulation studies evaluate the absorption, accumulation, and distribution of contaminants within organisms from environmental matrices, including soil, water, sediment, and air. These studies refine mass partitioning estimates by quantifying concentrations in organisms relative to their surrounding media, improving the accuracy of partitioning models.

Bioaccumulation factors (BAFs) measure the ratio of a contaminant's concentration in an organism to its concentration in the environment, accounting for exposure from multiple pathways, including diet (Government of Canada 2013). Field BAFs are calculated from water and biota samples, determining the ratio of tissue concentration to averaged water concentration, accounting for variability and lipid partitioning (USEPA 2000a). The K_{ow} and bioaccumulation data predict BAFs and model food web dynamics, incorporating trophic transfer and biomagnification (USEPA 2000a,b). Regulatory frameworks use BAFs to assess bioaccumulation potential. Canadian criteria define a substance as bioaccumulative if its BAF exceeds 5,000 or log K_{ow} is ≥5 (Government of Canada 1999), while British Columbia uses a threshold of 2,000 or log K_{ow} ≥4.5 (BC ENV 2023).

Bioconcentration factors (BCFs) quantify uptake from water, typically measured in laboratory settings (Government of Canada 2013). Laboratory BCFs measure steady-state tissue concentrations from water exposure (USEPA 2000a). Combined with food chain multipliers, these data account for additional dietary uptake, improving partitioning estimates (USEPA 2000a). Like BAFs, BCFs inform regulatory thresholds, with Canada applying the same 5,000 limit or a log K_{ow} ≥5 and British Columbia a 2,000 limit or a log K_{ow} ≥4.5 (Government of Canada 1999; BC ENV 2023).

Biota-sediment accumulation factors (BSAFs) calculate the ratio of a contaminant's concentration in an organism's lipid fraction to its concentration in sediment, normalized for organic carbon (Burkhard 2009). BSAFs connect sediment contaminants to bioaccumulation in aquatic organisms, informing sediment-biota partitioning (USEPA 2000b). These data refine models by linking sediment concentrations to biological uptake.

Plant uptake factors (PUFs) measure contaminant transfer from soil to plant tissues in terrestrial systems, calculated as the ratio of tissue to soil concentrations, assessing bioavailability (USEPA 2000b). PUFs improve partitioning estimates by quantifying soil-to-plant contaminant movement.

Mass partitioning models rely on predicted partition coefficients. Bioaccumulation studies provide field- and lab-based data from BAFs, BCFs, BSAFs, and PUFs to refine these predictions, reducing uncertainty and improving risk assessment and contaminant management.

Modelling

The laboratory, field, and literature data previously described are integrated into predictive models, including equilibrium partitioning models, contaminant transport models, and geochemical models, to simulate how contaminants move between soil, sediment, water, air, and biological systems under varying environmental conditions. For instance, equilibrium partitioning models utilize partitioning coefficients such as K_d (soil-water) or K_{ow} (octanol-water) to estimate the distribution of contaminants at steady-state conditions, providing insights into their mobility, bioavailability, and potential for remobilization under changes in temperature, pH, or organic content (USEPA 2008b). Specific tools like BIOSCREEN and BIOCHLOR, are screening-level models that simulate natural attenuation processes of hydrocarbons and chlorinated solvents in groundwater, respectively. These models incorporate dispersion, dilution and biodegradation

processes (Aziz et al. 2000). Contaminant transport models, such as Modular three-dimensional finite-difference ground-water flow model (MODFLOW), predict solute movement in groundwater by accounting for advection, diffusion, and dispersion, and are widely applied in hydrogeological assessments (Harbaugh 2005; Ohio Environmental Protection Agency [EPA] 2007). Geochemical models, like PHREEQC (PH [pH], RE [redox], EQ [equilibrium], and C [program written in Q]), analyse reactions affecting metal speciation and concentration, enhancing predictions of contaminant behaviour under site-specific conditions (Parkhurst & Appelo, 2013). Dynamic models, such as the Soil and Water Assessment Tool (SWAT), capture temporal changes in environmental conditions and contaminant levels, enabling long-term trend analysis and evaluation of remediation strategies (Arnold et al. 2012; Bloch et al. 2022).

Within Alberta's current framework, such as the Alberta Tier 1 and Tier 2 Guidelines, a modified version of the Domenico and Robbins analytical model is applied to predict contaminant transport in groundwater, using site-specific data to refine mass partitioning estimates by simulating advection, dispersion, and decay processes (AEPA 2024a,b). This model supports Tier 2 adjustments by providing a simplified yet effective tool to assess contaminant plume behaviour, enhancing risk assessments and remediation planning. The Johnson and Ettinger model accounts for diffusive transport processes through the vadose zone until vapour is proximally located to the building foundation, where advective processes dominate. In Alberta, the Johnson and Ettinger model is coupled with a simplified three-phase partitioning model to account for volatilization from soil and groundwater. This model accounts for attenuation of VOCs and SVOCs through the soil column due to adsorption; however, it does not account for degradation or dispersion. Model outcomes provide quantitative insights into contaminant distribution across phases, refining mass partitioning estimates for regulatory and management purposes.

Modelling as well as the integration of the aforementioned methods and principles contributes specific data on contaminant distribution across environmental phases, enabling the calculation of partitioning coefficients, and prediction of mobility and persistence. These techniques, applied individually or in combination, inform risk assessments and guide remediation strategies by providing a comprehensive understanding of contaminant behaviour.

Appendix A provides a case study that outlines the use of mass partitioning analyses to assess the transport, bioavailability, and risks of PCB contamination at the Hudson River PCBs Superfund Site in support of remediation strategies and risk reduction efforts.

4.4 Data Requirements

Supplementary data for mass partitioning analysis, exceeding a detailed CSM, are outlined below and categorized by type to enhance partitioning estimates across relevant media:

- Partitioning coefficients:
  - K_{oc} from soil/sediment organic carbon content (f_{oc}) to measure sorption affinity.
  - K_d from soil/sediment and groundwater interactions for site-specific sorption.
  - K_{aw} or Henry's Law Constant from water-vapour relationships to evaluate volatility.

- K_{ow} to assess bioaccumulation potential in organisms.
- K_{sa} from soil gas to determine vapour partitioning.

- Sorption/Desorption data:
  - Isotherms from soil/sediment batch tests to measure contaminants retention and release dynamics.
  - Desorption rates from porewater-soil/sediment tests to predict remobilization under changing conditions.
- Geochemical parameters:
  - pH, redox potential, temperature, and dissolved oxygen in groundwater, surface water, and porewater to influence contaminants solubility and speciation.
  - Ionic strength, hardness/alkalinity and salinity in water media to affect metal partitioning and mobility.
- Temporal data:
  - Seasonal sampling of groundwater, surface water, and vapour to capture dynamic partitioning trends.
  - Multi-depth soil/sediment sampling over time to track vertical distribution shifts.
- Phase distribution data:
  - NAPL composition in soil, sediment, or groundwater from core sampling to quantify free-phase mass.
  - Colloidal fractions in groundwater/porewater via filtration to assess transport in suspended phases.
  - Vapour concentrations from soil gas or headspace sampling for volatile contaminants distribution.
- Bioaccumulation data:
  - BAFs/BCFs from biota (e.g. fish, plants) sampling in water/sediment systems to link media to ecological risks.
  - BSAFs from sediment-biota tests to quantify organic contaminants uptake.
  - PUFs from soil-plant studies to measure terrestrial bioavailability.
- Media-Specific needs:
  - Soil: Moisture content, f_{oc} and grain size distribution to refine sorption capacity estimates.
  - Sediment: Organic matter and clay content to assess binding potential for contaminants.
  - Groundwater: Hydraulic conductivity from well tests to support transport modelling.
  - Surface Water: Flow rates and dilution factors to evaluate plume dispersion.
  - Porewater: Dissolved contaminants concentrations via lysimeters[3] for interstitial water partitioning.
  - Vapour: Depth-to-source measurements to assess intrusion or atmospheric dispersion risks.

[3] A lysimeter is a container filled with soil that measures water and material movement through the soil.

- Biota: Tissue residue data to quantify trophic transfer and biomagnification.

4.5 Applications

Table 4-1 outlines key applications of mass partitioning at contaminated sites. Each application demonstrates how partitioning data are integrated into site management processes to assess risks, guide remediation strategies, ensure regulatory compliance, and verify ongoing site stability. Table 4-2 and

Table 4-3 outline site types where mass partitioning analysis is either beneficial or unsuitable.

Table 4-1: Applications of Mass Partitioning in Contaminated Site Management

Application	Description	Key Uses
Site Characterization	Mass partitioning quantifies contaminant distribution across environmental phases (soil, water, soil vapour, air, biota) to identify concentration gradients and phase-specific behaviour.	• Determine contaminant mobility and persistence. • Identify primary environmental phases of concern. • Map contaminant distribution patterns.
Risk Assessment	Mass partitioning informs exposure pathways by identifying how contaminants are distributed between phases and their potential bioavailability.	• Assess human and ecological exposure risks. • Identify bioavailable contaminant fractions. • Prioritize high-risk exposure pathways.
Remediation Planning	Understanding mass partitioning guides remediation strategies by predicting contaminant retention, mobility, and transfer between environmental media.	• Design targeted remediation approaches. • Predict contaminant response to remediation efforts. • Select appropriate remedial technologies. • Inform selection of technologies such as pump-and-treat, soil vapour extraction, in situ chemical oxidation/reduction, or thermal desorption based on partitioning behaviour.
Predictive Modelling	Mass partitioning coefficients (e.g. K_d, K_{oc}, K_{ow}) are used in models to simulate contaminant transport, transformation, and long-term environmental behaviour.	• Predict contaminant fate and transport. • Evaluate contaminant stability under varying conditions. • Assess long-term remediation outcomes.
Vapour Intrusion Assessment	Mass partitioning helps predict the extent of vapour migration.	• Evaluate risks of volatile contaminants migrating into indoor air. • Inform the design of mitigation measures, such as vapour barriers or sub-slab depressurization systems.
Regulatory Compliance	Mass partitioning data provide quantitative evidence of contaminant behaviour, supporting regulatory assessments and demonstrating compliance.	• Provide defensible contaminant distribution data. • Demonstrate site-specific compliance with guidelines. • Support closure applications.
Monitoring and Verification	Mass partitioning principles are used to evaluate changes in contaminant distribution post-remediation, assessing stability and identifying rebound potential.	• Track contaminant redistribution trends Verify long-term containment effectiveness. • Identify potential for recontamination.

Table 4-2: Relevant Sites for Mass Partitioning Analysis

Type of Site	Reason	Limitations
Sites with single contaminant sources	Facilitates accurate assessment of contaminant partitioning across media (e.g. soil, sediment, water, air).	Does not account for interactions between multiple contaminants or complex degradation pathways.
Hydrocarbon-contaminated sites (e.g. BTEX, PHCs, PAHs)	Hydrocarbons exhibit predictable partitioning behaviour between soil, water, and air.	Partitioning behaviour can still be influenced by site-specific factors such as temperature, organic matter, and microbial activity.
Sites with volatile contaminants	Volatile contaminants partition readily into air, water, and soil phases.	Volatilization rates can vary due to site-specific conditions such as temperature, soil properties, and moisture content.
Sites with groundwater contamination	Mass partitioning helps determine the distribution of contaminants between dissolved and sorbed phases.	Does not fully capture the effects of complex hydrogeological conditions, advection, and biodegradation.
Gas plants and well pads	Often have contaminants (e.g. PHCs, sulphur compounds, salts and organic compounds) that partition into multiple phases, enabling comprehensive analysis.	Presence of mixed contaminants, aging hydrocarbons, and degradation byproducts can complicate partitioning predictions.
Sites with well-defined hydrology	Hydrology influences the partitioning behaviour of contaminants, making results more interpretable.	Changes in groundwater flow, seasonal variations, and subsurface heterogeneity can introduce uncertainties.
Sites with multiple media impacts	Useful in evaluating partitioning between soil, sediment, groundwater, surface water, vapour and biota for cross-media assessment.	Increased complexity in modelling due to interactions between different media and environmental conditions.
Non-complex contaminant mixtures	Useful when contaminants have well-understood partitioning coefficients. Allows for a straightforward assessment of the distribution and behaviour of individual contaminants across different media, aiding predictions of mobility, bioavailability, and environmental risks without considering complex substance interactions.	May oversimplify the interactions between contaminants and environmental media by assuming uniform behaviour across the mixture, which can overlook variations in individual contaminant properties, leading to less accurate predictions of mobility, bioavailability, and environmental risks.

Table 4-3: Unsuitable Sites for Mass Partitioning Analysis

Type of Site	Reason
Sites with immiscible phases (NAPLs not partitioning significantly)	Free-phase contaminants typically do not follow equilibrium-based partitioning, requiring multiphase flow modelling instead.
Sites with unknown or comingled contaminant sources	Difficult to apply when the contamination sources are poorly defined or mixed.
Sites with predominantly inorganic contamination	Inorganics, like heavy metals, do not partition predictably between phases like organic compounds, being more influenced by chemical reactions and site-specific conditions than equilibrium distribution.
Complex contaminant mixtures with limited data	Challenging when partitioning coefficients for key contaminants are unavailable.

Type of Site	Reason
Sites with highly heterogeneous geology	Reduced accuracy in complex subsurface environments with variable properties.
Multi-source contamination with extensive cross-interaction.	Unsuitable for cases where partitioning is overshadowed by external interactions.

4.6 Relationship to Alberta Policy

4.6.1 Current Status

The use of mass partitioning of contaminants as a decision-making tool in contaminated sites investigation, remediation and risk assessment is currently recognized within current Alberta policy as summarized below.

- The standard Tier 1 and Tier 2 models for groundwater transport and vapour intrusion rely on mass partitioning calculations to estimate soil to groundwater transport and soil/groundwater to vapour transport (AEPA 2023; 2024a; 2024b). Alternative models are also permitted within risk assessment with appropriate consultation (AEP 2023).
- While not explicitly documented within Alberta written policy and guidance documents, mass partitioning has precedent of being an acceptable line of evidence to inform ROAs / feasibility studies.
- Risk assessments are expected to evaluate both direct and indirect exposure pathways under current conditions and in future (AEP 2023; AEPA 2023). Existing guidance (AEP 2023) references use of cross-media partitioning (e.g. mass partitioning) to quantify current and future exposures considering contaminant fate and transport, and receptor exposure pathways.
- Risk management plans are required to explicitly identify site-specific conditions where contaminant concentrations could affect how contaminants partition in environmental media (AEP 2017). While this does not explicitly specify that mass partitioning calculations are required, it is inferred that mass partitioning calculations could be used to address this requirement.
- While not explicitly documented within Alberta written policy and guidance documents, mass partitioning may be incorporated in complex fate and transport models. Complex fate and transport models are documented as an acceptable line of evidence to support risk assessment and long-term risk management (AEP 2023).

4.6.2 Gaps in Alberta Policy and Opportunities for Improvement

There are gaps in Alberta's written policy and guidance about what mass partitioning models and measurement methods AEPA and AER will accept, limitations on when mass partitioning calculations must be used versus when site-specific measurements are sufficient and what input parameters are acceptable. Furthermore, Alberta has limited the ability of practitioners to use published physico-chemical parameters (including partitioning coefficients) not included in Tier 1 and Tier 2 guidance documents (AEPA 2024a; 2024b). To address these gaps, it would be beneficial to provide formal written policy and/or guidance that describes:

- What mass partitioning models are acceptable;

- What mass partitioning measurements are acceptable, particularly when considering many methods to estimate partitioning coefficients and/or bioavailability would be completed by laboratories without accreditation for said methods (e.g. research facilities, universities);
- What site-specific conditions preclude the use of mass partitioning calculations in support of site investigation, remediation and/or risk assessment;
- What input parameters are acceptable in mass partitioning calculations including, as appropriate:
  - Use of literature/default partitioning coefficients;
  - When site-specific data must be collected and what methods will be considered applicable; and
  - How to approach situations where site-specific information is unavailable or is impracticable to collect/measure.

Of particular importance to practitioners is more clearly defined options for use of published physico-chemical properties such as K_{oc}. The current written policy generally precludes the use of published physico-chemical properties that are not contained within the Tier 1 and Tier 2 guidelines (AEPA 2023; 2024a; 2024b). Providing written policy and/or guidance on the methods and key assumptions that are acceptable to AEPA and AER for estimating total mass would provide consistency in these evaluations, limit rework and minimize potential for both submission returns and SIRs.

4.7 Costing

The following table provides an estimated cost breakdown for conducting a mass partitioning analysis for a standard oil and gas lease in Alberta (see Section 1.3.1 for definition and assumptions). This analysis aims to evaluate the distribution of contaminants among different phases—solid, aqueous, and vapour—within the soil and groundwater.

Table 4-4: Estimated Cost for a Mass Partitioning Analysis at a Standard Oil and Gas Lease

Task	Description	Cost Estimate
Project Planning and Data Review	Review existing CSM (soil/groundwater [GW] data from 10–20 wells), plan 10 soil samples and GW sampling; coordinate logistics (lab, equipment).	$2,250 - $3,000
Partitioning Coefficients	Measure K_d (metals) and $K_{oc} \times f_{oc}$ (organics) via lab analysis of 10 new soil samples and groundwater from 10 existing wells; literature values for K_{aw}, K_{ow}, K_{sa}; batch tests for site-specific sorption.	$5,000 - $7,000
Sorption/Desorption Data	Conduct batch tests on five soil samples to generate sorption/desorption isotherms for 20 COPCs (PHCs, PAHs, metals, salinity, VOCs).	$2,500 - $4,000
Geochemical Parameters	Measure pH, redox, temperature, and dissolved oxygen (DO) in groundwater from 10 wells; lab analysis of ionic strength and salinity; 1-day field effort with handheld meters and sample collection.	$3,500 - $4,500
Phase Distribution - NAPL (if applicable)	Assess NAPL composition in soil/GW via core sampling (five boreholes) and lab analysis; targets PHCs/VOCs NAPLs not fully detailed in the CSM.	$7,500 - $10,000
Media-Specific - Soil	Measure moisture content and grain size distribution for 10 new soil	$500 - $1,000

	samples; include lab sieve analysis and moisture tests.	
Media-Specific - Groundwater	Assess hydraulic conductivity via slug tests at 5 wells; 1-day field effort with equipment rental and analysis.	$2,500 - $3,500
Field Labor and Equipment	Deploy field crew (two technicians, two days) for soil sampling, GW measurements, and NAPL coring; equipment rental (coring rig, meters) and vehicle access; assumes year-round access.	$10,000 - $12,000
Laboratory Analysis	Analyse 10 new soil samples for 20 COPCs (PHCs, PAHs, metals, salinity, VOCs) to quantify phase-specific concentrations (dissolved, sorbed); excludes duplicated physical properties.	$5,000- $6,250
Data Compilation and Reporting	Compile data, calculate partitioning distributions, and prepare associated report.	$3,000 - $4,500
Project Management	Oversee field activities (two days), lab submissions, and reporting; includes scheduling, QA/QC, and client/regulatory communication.	$3,000 - $4,500
Total Estimated Cost		**$44,750 - $60,250**

These estimates are approximate and can vary based on site-specific conditions, regional labor rates, and the complexity of the contamination. Costs will be reduced if data are collected concurrently with CSM development and/or execution of other field programs.

4.8 Summary

Mass partitioning analysis offers a comprehensive, cost-effective approach to assess contaminated sites by quantifying how contaminants distribute across environmental media (e.g. soil, sediment, groundwater, air) and phases (e.g. sorbed, dissolved, vapour). Mass partitioning leverages data from routine site characterization coupled with specialized analysis to predict contaminant behaviour, fate, and transport with minimal additional expense. This method enhances risk assessment, remediation planning, and pollution control by integrating site-specific partitioning coefficients and models, making it adaptable for diverse sites and supportive of other mass-based techniques when further investigation is needed.

5. Mass Flux and Mass Discharge Quantification

5.1 Description

Mass flux (J) measures the amount of a chemical, such as a contaminant or additive, moving through a specific cross-sectional area of a transport medium, like groundwater or soil vapour over time. It integrates two key factors of a contaminant plume: the concentration of the contaminant in the groundwater and the velocity of groundwater flow through that area (ITRC 2010a; CRCCARE 2016). As a vector quantity, mass flux has both magnitude and direction, expressed in units of mass per area per time (e.g. kg/m²/s). Calculating mass flux provides a detailed view of contaminant movement by accounting for spatial variations in concentration and flow velocity across a plume.

Mass flux estimates provide a more detailed characterization of a contaminated site than typical monitoring networks, which focus only on contaminant concentrations (Feenstra, Cherry, and Parker 1996). Mass flux quantifies the rate at which a contaminant moves through a defined cross-sectional area of a transport medium, such as groundwater or soil vapour (see Figure 5-1). While conventional monitoring defines plume boundaries and concentration trends, this approach can often miss areas of significant flux due to variations in chemical concentrations and groundwater velocities within the plume. As such, calculating mass flux, which integrates the variability of concentration and velocity across the plume, offers a more thorough site assessment. Additionally, mass flux values at different times and locations capture the combined effects of physical, chemical, and biological processes on contaminants. This detailed insight improves the CSM and supports remediation decisions by identifying source strength, aquifer heterogeneity, and treatment zones (Nichols and Roth 2004, Basu et al. 2006). However, measuring mass flux can be challenging because it varies across a control plane due to fluctuations in contaminant concentrations and groundwater flow (ITRC 2010a). Multiple measurements are often required to effectively characterize these variations, particularly in dissolved contaminant plumes. Because mass flux is assessed over a small area relative to the entire plume, it may not fully represent overall plume behaviour under changing conditions (ITRC 2010a).

Mass discharge (Md) quantifies the total mass of a solute, such as a contaminant, migrating from a source or passing through a control plane, without being confined to a specific area. As a scalar quantity, it is measured in units of mass per time (e.g. kg/s; ITRC 2010a; CRCCARE 2016). Mass discharge is estimated by measuring contaminant concentrations and groundwater fluxes along a transect perpendicular to groundwater flow, as shown in Figure 5-1 (Looney et al. 2006; ITRC 2010a). Unlike mass flux, which varies spatially across a control plane, mass discharge represents the total flux across the entire plane, providing a single, integrated value that is spatially uniform, varying only with time since it reflects a single integrated value for the entire plane. This makes it a preferred metric for characterizing the overall rate of contaminant release from a source and the total mass moving through a plume (ITRC 2010a).

Estimating mass discharge is often cost-effective and valuable for risk assessments and transport modelling. By providing an upper limit of the contaminant load, mass discharge offers a conservative estimate that accounts for variability and supports regulatory prioritization (ITRC 2010a; CRCCARE 2016). Mass discharge is widely applied in regulatory contexts, such as the Record of Decision (ROD) for the Well 12A federal superfund site in Washington state which included a mass discharge interim goal (USEPA 2009). Surface water regulations, such as the National Pollutant Discharge Elimination System (NPDES), Water Quality Based Effluent Limits (WQBELs), and Total Maximum Daily Loads (TMDLs) use mass discharge principles to assess the potential cumulative effects of wastewater discharge to waterbodies.

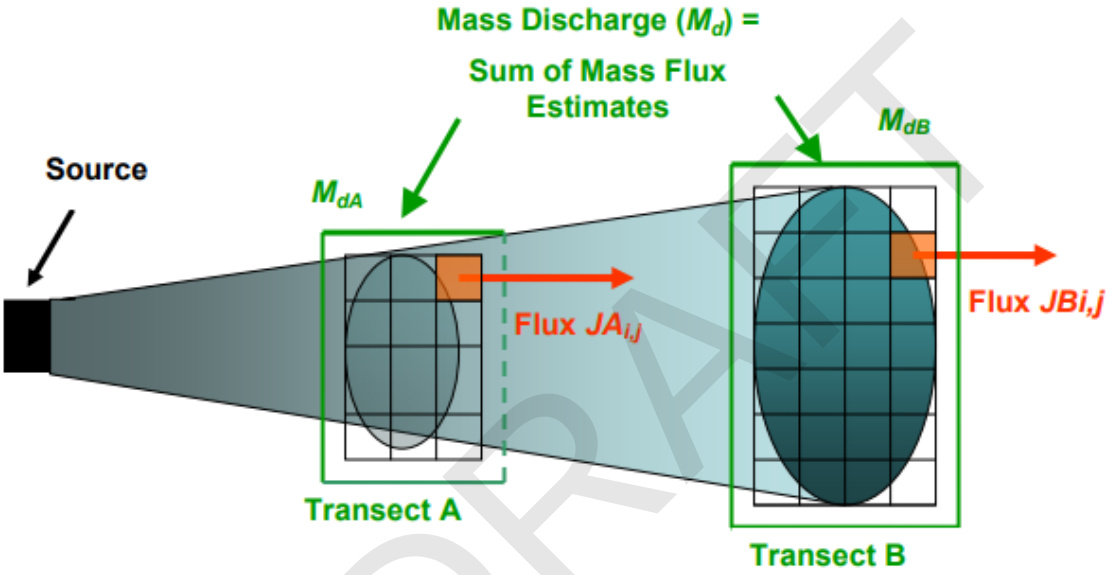

Figure 5-1: Concepts of Mass Flux (J) and Mass Discharge (M_d).
Mass flux measures the rate at which contaminant mass moves through a specific area of a plane per unit of time (e.g. grams [g] per day [d] per square meter [m^2]). Each segment of a transect corresponds to the flux for that specific area (i.e. JAi,j and JBi,j). Mass discharge represents the total contaminant mass moving across the entire area of the transect (e.g. g/d), calculated by summing the fluxes of the segments within a transect. This figure illustrates the comparison of mass discharge values (i.e. M_{dA} and M_{dB}) measured at varying distances from a source. Such comparisons are valuable for evaluating site conditions, including determining natural attenuation rates and assessing contaminant behaviour over distance. Republished from: ITRC 2010a.

Considering mass flux and mass discharge data enhances remediation decisions by offering insights that go beyond concentration data. These metrics help assess source strength, aquifer heterogeneity, exposure risks, attenuation capacity, and treatment zones, while also supporting the establishment of remedial goals and regulatory prioritization based on source strength and receptor threats (ITRC 2004, 2008a, 2008b). Although concentration-based guidelines dominate regulatory frameworks, mass flux and mass discharge have been applied in several regulatory contexts. Their use improves evaluation of groundwater extraction systems and determines the effectiveness of natural attenuation processes in reducing contaminant mass flux. These examples

highlight the potential for broader adoption of mass flux and mass discharge in contaminated site management (ITRC 2010b).

The following table compares mass flux and mass discharge across key characteristics, illustrating their distinct roles in understanding and managing contaminant plumes.

Table 5-1: Summary Table: Mass Flux vs. Mass Discharge

Aspect	Mass Flux (J)	Mass Discharge (Md)
Definition	Measures contaminant transport per unit area over time	Measures total contaminant mass passing through a control plane over time
Units	Mass per area per time (e.g. kg/m²/s)	Mass per time (e.g. kg/s)
Type	Vector quantity (dependent on direction and magnitude)	Scalar quantity (direction-independent)
Spatial Considerations	Integrates concentration and velocity over a small area	Integrates concentration and flux across an entire transect
Variability	Varies spatially across a plume	Spatially uniform, varies only with time
Advantages	Detailed local plume characterization	Comprehensive view of total contaminant load
Challenges	Requires multiple measurements for accuracy	Less detail on spatial variations

5.2 Media Considered

Mass flux and mass discharge analyses primarily focus on two key environmental media as transport mediums for contaminants, which are outlined below:

- **Groundwater:** Groundwater is the more commonly assessed medium using mass flux and mass discharge, as both methods quantify the movement of dissolved contaminants, such as hydrocarbons or chlorinated solvents, through aquifers by integrating contaminant concentrations with groundwater flow velocities (ITRC 2010a; CRCCARE 2016).
- **Soil Vapour:** Soil vapour is considered in contexts where volatile contaminants, such as VOCs, migrate through the unsaturated zone, allowing mass flux to capture the rate of vapour-phase transport across a defined cross-sectional area (ITRC 2010a).

5.3 Approach

Mass flux of a contaminant is mathematically determined by multiplying the contaminant concentration in groundwater by the groundwater flux (ITRC 2010a; CRCCARE 2016). This relationship can be expressed using the formula:

$$J = q_0 * C = -K * i * C \qquad \textbf{Equation 5-1}$$

where:

J = contaminant mass flux (e.g. g/m^2/day)

q_0 = groundwater flux or Darcy velocity (e.g. flow rate/area; [m^3/day]/m^2 or m/day)

C= contaminant concentration (e.g. mg/volume)

K = saturated hydraulic conductivity (e.g. m/d)

i = hydraulic gradient, dimensionless (e.g. m/m)

Contaminant mass discharge is calculated by integrating the mass flux values across a defined transect area, summing the contributions from segments of the plane, as express by:

$$M_d = \int_A J dA \qquad \textbf{Equation 5-2}$$

where:

M_d = mass discharge (e.g. g/d)

A = area of the control plane (e.g. m^2)

J = spatially variable contaminant flux, as defined in Equation 2-1

dA = the differential area element across the control plane (e.g. m^2) (ITRC 2010a; CRCCARE 2016).

The following provides a description of each of the primary methods used to assess mass flux and mass discharge at contaminated sites. Table 5-2 compares these methods, including their data requirements, objectives, strengths, challenges, and preferred applications.

Transect Method

Transect methods involve measuring the movement of contaminants through groundwater by collecting data along a plane, or transect, positioned perpendicular to the direction of groundwater flow. This method uses a network of monitoring wells or multilevel samplers (MLSs) to capture variations in contaminant concentrations and flow velocities across the plume's cross-section (ITRC 2010a). The required data include contaminant concentrations at multiple points and the specific discharge, calculated as the product of hydraulic conductivity and hydraulic gradient. Mass flux is determined for each sampling point and mass discharge is computed by integrating these fluxes across the entire transect area. In practice, transect methods are used to assess plume stability, evaluate natural attenuation rates, and identify high-priority treatment zones, often with tools like the Mass Flux Toolkit (ITRC 2010a), to process data from detailed sampling grids, providing a comprehensive picture of contaminant movement and aiding in remediation planning.

Well Capture / Pumping Test Method

Well capture or pumping test methods estimate mass discharge by extracting groundwater through a pumping well and measuring the total contaminant mass removed over time, offering a direct assessment of contaminant load leaving a site. This approach requires data on the pumping rate (Q), typically in gallons per minute, and the average contaminant concentration in the extracted water (C_{sw}), with mass discharge (Md) calculated as $Md = Q \cdot C_{sw}$ (ITRC 2010a). Additional data, such as the capture zone boundaries of the pumping system and aquifer

properties, may be needed to refine estimates using techniques like integral pump tests (IPTs) or modified IPTs (MIPTs). The method is commonly applied at sites with existing pump-and-treat systems to evaluate source zone depletion or assess mass discharge to receptors like supply wells, integrating variability across the capture zone into a single, practical measurement that informs remediation performance and receptor protection strategies (ITRC 2010a).

Passive Flux Meters

Passive flux meters are devices installed in monitoring wells to directly measure groundwater and contaminant fluxes over an extended period without active pumping. This approach provides a time-integrated snapshot of plume dynamics (ITRC 2010a). Passive flux meters comprise a cylindrical sorbent matrix, such as activated carbon, infused with tracers that are released in proportion to the groundwater flow rate, while simultaneously capturing and retaining contaminants on the sorbent surface. Data required include the residual tracer mass and captured contaminant mass after retrieval, which are analysed to calculate specific discharge and mass flux at discrete vertical intervals (ITRC 2010a). Passive flux meters are used to assess seasonal variability in flux, monitor bioremediation or natural attenuation processes, and evaluate risks near receptors, offering a non-invasive approach that captures detailed flux distributions within a well, which can then be scaled to estimate plume-wide mass discharge with multiple installations.

Transects Based on Isocontours

Transects based on isocontours estimate mass discharge by leveraging existing concentration data from monitoring wells, plotted as isocontour lines (equal concentration boundaries) perpendicular to groundwater flow, without requiring new sampling transects. This method relies on historical contaminant concentration data from the monitoring network at a site, and an estimated Darcy velocity, derived from hydraulic conductivity and gradient measurements or assumptions (ITRC 2010a). Mass discharge is calculated by integrating concentrations with flow rates across the plume width along these contours. It is used for preliminary assessments, site prioritization, or retrospective analysis of remediation performance when resources for new fieldwork are limited (ITRC 2010a). By leveraging existing data, this approach provides a cost-effective, albeit less detailed, estimate of contaminant load that can guide initial decision-making or refine the CSM.

Solute Transport Models

Solute transport models use numerical or analytical simulations to estimate mass flux and discharge by modelling groundwater flow and contaminant transport across a site, based on a computational grid of site-specific parameters (ITRC 2010a). These models, such as MODFLOW for flow and MT3DMS for transport, require extensive input data, including hydraulic conductivity, hydraulic gradient, contaminant concentrations, porosity, and defined boundary conditions, often calibrated with field measurements. The models compute spatially and temporally variable flux estimates, integrating these parameters to predict plume behaviour and calculate mass discharge across defined transects or boundaries. They are used to forecast remediation outcomes, assess long-term risks to downgradient receptors, and test hypothetical scenarios for remedial design,

offering a powerful tool for comprehensive site management when paired with field data for validation and refinement (ITRC 2010a).

Thermal Tracer Method (Temperature-Based Mass Flux Estimation)

The thermal tracer method estimates mass flux and discharge by analysing temperature variations in groundwater caused by mixing processes, using heat as a natural tracer to infer flow rates without directly quantifying contaminant concentrations (Anderson 2005). This approach requires data on temperature profiles across a site, typically collected using high-resolution temperature sensors or borehole thermistors in wells, along with known or assumed thermal properties of the aquifer (e.g. thermal conductivity, specific heat capacity) and background temperature gradients. Rather than measuring contaminant concentrations, it relies on existing concentration data paired with temperature-derived flow estimates. Specifically, mass flux is determined by combining the groundwater flow rate, which is estimated from temperature changes using principles like heat transport and mixing processes, with a known or modelled contaminant concentration (Anderson 2005). Mass discharge is then calculated by summing these mass flux values across a designated control plane. The method is used in settings where temperature contrasts—such as those from surface water infiltration, geothermal gradients, or artificial heat sources—reveal flow patterns, aiding in plume delineation, recharge assessment, or mass discharge estimation near receptors. This approach offers a unique, indirect approach to flux assessment when traditional concentration sampling is impractical or supplementary flow data is needed.

Isolation (Static) Flux Chambers (Vapour Flux Estimation)

Isolation flux chambers measure diffusive vapour flux by enclosing a defined surface area, isolating it from external influences such as wind or atmospheric pressure changes (USEPA 1993). A high-uptake-rate passive absorptive sampling tube, containing sorbents like activated carbon or polymer resins, is placed inside the chamber to capture VOCs via molecular diffusion over a sampling period (e.g., 24 hours). The collected VOC mass is analyzed using gas chromatography-mass spectrometry (GC-MS) to determine the emission rate, expressed as flux (µg/m²/min). This method is cost-effective, requires minimal equipment, and is well-suited for long-term monitoring of diffusive emissions from contaminated surfaces (USEPA 1993).

Dynamic Flux Chambers (Vapour Flux Estimation)

Dynamic flux chambers actively measure vapour flux by introducing a continuous flow of clean carrier gas (e.g. nitrogen or zero-air) into a chamber enclosing the surface (Gao et al. 1997; Almand-Hunter et al. 2015). The carrier gas mixes with emitted vapour, and the exhaust gas is sampled in real time, typically analyzed via GC-MS to calculate the emission rate (e.g. µg/m²/min). This method is widely used in environmental monitoring for high-precision, real-time measurements, particularly for assessing transient or variable emission sources (Gao et al. 1997; Almand-Hunter et al. 2015).

Appendix B provides a case study that focuses on the use of a mass flux based approach to evaluate the short-term and localized aquatic impacts of molybdenum containing water released in southeast Alberta, while incorporating a weight of evidence framework to assess risks and confirm the resilience of the aquatic environment.

Table 5-2: Comparison of Methods for Measuring Mass Flux and Mass Discharge (derived from ITRC 2010a and Anderson 2005)

Approach	Description	Data Required	Purpose	Strengths	Challenges	Primary Uses
Transect Methods	Estimates contaminant mass flux along a cross-sectional transect of the plume by installing monitoring points and collecting concentration and flow data.	Groundwater contaminant concentrations. Groundwater flow velocities. Transect layout (spacing and number of monitoring points).	Evaluate spatial distribution of flux. Identify high-flux zones for targeted remediation. Refine CSM.	High spatial resolution. Identifies high-flux zones.	Requires high-resolution characterization data. Potential for interpolation errors if the sampling density or spatial variability is not adequately captured. Cost-intensive for sampling and analysis.	Accurately map and quantify the total contaminant mass discharging into a receiving environment using high spatial resolution data. Characterizing plumes, identifying remediation zones, and estimating natural attenuation.
Well Capture / Pump Tests	Groundwater is pumped from one or more wells to measure total contaminant mass discharge and groundwater flow directly.	Total volume of groundwater extracted. Contaminant concentrations in the extracted water. Well placement and pumping rates must be such that the full extent of the plume is captured.	Directly measure total contaminant mass discharge at a specific location or across a specific area. Confirm remediation effectiveness by monitoring changes in mass discharge over time.	Reduces interpolation error compared to transect methods. High certainty of capturing contaminant flux at the selected location. Effective for compliance monitoring and plume characterization.	Requires significant infrastructure, including wells and pumps (e.g. larger diameter wells are useful for higher pumping rates or longer-term extraction). Generates large volumes of water that may require treatment and disposal. Does not provide spatial distribution data within the plume and is limited by the effectiveness of well placement and selected pumping rates.	Provides for direct measurement of total mass discharge at specific locations. Assessing total mass discharge, evaluating pump-and-treat systems, and verifying remediation progress.
Passive Flux Meters	Directly measures contaminant and water flux over time using passive flux meters that are placed in wells for a set duration. The devices absorb contaminants and measures the volume of water passing through the well. Data collected are analysed to calculate both contaminant and groundwater flux.	Device deployment data, including placement and duration of measurements. Absorbed contaminant mass and water flux (rate of groundwater flow through a unit area perpendicular to the flow direction) measurements.	Measure localized contaminant transport rates. Provide continuous data over the deployment period.	Simple deployment and retrieval. Disturbance to the site is minimal and no purge water is generated. Reduces the need for frequent sampling or monitoring.	Limited to the area immediately surrounding the well. May require site-specific calibration to account for varying conditions. Does not provide high spatial resolution data across the plume unless deployed in multiple locations.	Quick, low-disturbance approach for localized measurements; long-term, passive monitoring. Monitoring post-remediation fluxes and tracks mass reduction pre/post-treatment.
Transects Based on Isocontours	Estimates mass discharge indirectly by multiplying groundwater flow rates and contaminant concentrations collected from monitoring wells or isocontours.	Groundwater flow rates and hydraulic conductivity data. Contaminant concentrations from monitoring wells or isocontour maps.	Provides a cost-effective means to estimate mass discharge. Useful for sites with extensive existing monitoring data.	Leverages existing data, reducing the need for new fieldwork. Useful for initial estimates of mass discharge. Cost-effective.	Highly dependent on the quality and spatial resolution of input data. May underestimate discharge if high-flux zones are not adequately sampled/characterized. Less accurate than other approaches.	Provides cost-effective estimates of mass discharge where detailed field work is not needed. Preliminary estimates of mass discharge; supporting plume stability analysis.
Solute Transport Models	Numerical solute transport models use input data such as groundwater flow rates, contaminant concentrations, and site-specific hydrogeological parameters to simulate contaminant transport and calculate mass discharge.	Contaminant concentration data. Groundwater flow rates and hydraulic conductivity values. Site-specific parameters, such as porosity and dispersion coefficients.	Predict future plume behaviour under different scenarios. Evaluate the effectiveness of natural attenuation and remediation strategies.	Flexible and capable of simulating complex systems. Useful for assessing long-term plume behaviour and risks.	Requires extensive, high-quality input data. Complex to set up and calibrate, especially for heterogeneous aquifers. Results are model-dependent and may not fully reflect site-specific conditions.	Provides long-term predictions and input into development of remediation strategies.
Thermal Tracer Method	Uses temperature mixing to estimate groundwater discharge, paired with measured concentration.	Temperatures (groundwater, surface water, point of groundwater and surface water mixing), concentration, total flow (optional), location and extent of mixing zone.	Estimate bulk mass discharge at discharge interfaces (e.g. streams).	Non-invasive; leverages natural thermal signals; cost-effective for large areas.	Requires thermal contrast; limited to mixing zones; sensitive to thermal noise.	Groundwater contaminant loading to surface water (e.g. rivers, lakes).
Isolation (Static) Flux Chamber	Encloses a surface area with a passive absorptive sampling tube (e.g. containing activated carbon or polymer resins) to capture VOCs via molecular diffusion over a set period. VOC mass is analysed using GC-MS to calculate flux.	VOC mass collected, sampling duration, surface area, GC-MS analysis results.	Quantify diffusive VOC emissions from soil, waste, or liquid surfaces to assess contamination and vapour intrusion risks.	Cost-effective, minimal equipment, no power required, suitable for long-term monitoring.	Limited to diffusive flux, slower data collection, less precise for variable emissions.	Long-term monitoring of stable, diffusive VOC emissions at contaminated sites, especially in remote areas.

Approach	Description	Data Required	Purpose	Strengths	Challenges	Primary Uses
Dynamic Flux Chamber	Encloses a surface area and introduces a continuous flow of clean carrier gas (e.g. nitrogen or zero-air) to mix with emitted vapours. Exhaust gas is sampled in real-time and analysed via GC-MS to calculate flux (µg/m²/min).	Carrier gas flow rate, VOC concentrations in exhaust, surface area, GC-MS analysis results.	Measure real-time VOC emissions to assess transient or variable sources and support immediate risk evaluations.	High precision, real-time data, effective for variable emissions, adaptable to different surfaces.	Requires power, complex setup, higher cost, sensitive to carrier gas quality and flow consistency.	Real-time assessment of VOC emissions, particularly for dynamic or heterogeneous sources at contaminated sites.

5.4 Data Requirements

Data requirements for the six primary approaches used to assess mass flux and mass discharge, beyond those of a typical CSM, are outlined below. Data requirements have been synthesized from ITRC (2010) for the transect, well capture / pumping test, passive flux meter, transects based on isocontours, and solute transport model methods, while the thermal tracer method is described by Anderson (2005).

5.4.1 Transect Method

- Contaminant Concentrations (C): Measured at multiple points along one or more transects perpendicular to groundwater flow. Requires groundwater samples from wells, MLSs, or direct-push devices (e.g. Waterloo Profiler) at discrete vertical and horizontal intervals. Typically, in units of mass/volume (e.g. mg/L).
- Groundwater Flux (q): Specific discharge ($q=K \cdot i$) at each sampling point:
  - Hydraulic Conductivity (K): Estimated via slug tests, pumping tests, or grain size analysis at each point or representative zones. Units: length/time (e.g. m/day).
  - Hydraulic Gradient (i): Derived from water level measurements in piezometers or wells along the transect, often requiring a network of at least three points to define flow direction and magnitude. Dimensionless (m/m).
- Transect Geometry: Cross-sectional area (A) of each sampling segment, defined by horizontal spacing (i.e. lateral distance between sampling points along the transect, defining the width of each segment) and vertical intervals (i.e. depth increments sampled within the aquifer's saturated thickness, defining the height of each segment). Units: area (e.g. m^2).
- Temporal Data (Optional): Repeated measurements to assess seasonal variability, plume stability and/or attenuation over time.
- Collection Methods: Drilling wells, installing MLSs, or using direct-push tools; hydraulic tests for K and head measurements for i.

5.4.2 Well Capture / Pumping Test Methods

- Contaminant Concentrations (C): Average concentration in extracted water, measured via sampling during pumping. Requires multiple samples over time to account for stabilization or transients. Units: mass/volume (e.g. mg/L).
- Pumping Rate (Q): Volumetric flow rate of extracted groundwater, measured with flow meters (e.g. L/day). For IPTs, multiple rates are tested.
- Capture Zone Definition:
  - Drawdown Data: Water level declines in observation wells to confirm plume capture (e.g. change in hydraulic head divided by the horizonal distance of two points). Units: length (e.g. m).
  - Aquifer Thickness (b): Saturated thickness intersected by the well screen. Units: length (e.g. m).
- Hydraulic Parameters (Optional for IPT): Transmissivity ($T=K \cdot b$) and storativity from pumping test analysis to extrapolate total plume discharge. Units: Transmissivity in m^2/day; storativity is dimensionless.

- Collection Methods: Pumping wells, flow meters, sampling equipment, and observation wells for drawdown.

5.4.3 Passive Flux Meters

- Contaminant Mass Sorbed: Mass of contaminants captured by the passive flux meter's sorbent (e.g. activated carbon), analysed post-retrieval in segmented intervals. Units: mass (e.g. mg).
- Tracer Loss: Initial and residual tracer mass (e.g. alcohols) in the passive flux meter, measured before and after deployment to calculate groundwater flux (q). Units: mass (e.g. mg).
- Deployment Duration (t): Time passive flux meters are exposed to groundwater flow. Units: time (e.g. days).
- Well Geometry: Screen length and diameter to match passive flux meter's dimensions. Units: length (e.g. m).
- Sorbent Properties: Retardation factors and sorption capacity, typically lab derived.
- Collection Methods: Installation of passive flux meters in wells, retrieval, and lab analysis (e.g. gas chromatography).

5.4.4 Transects Based on Isocontours

- Contaminant Concentrations (C): Historical or current concentrations from gridded monitoring wells, interpolated into isocontour maps. Units: mass/volume (e.g. mg/L).
- Groundwater Flux (q) – Average specific discharge across the transect:
  - Hydraulic Conductivity (K): Regional or site-averaged value. Units: length/time (e.g. m/day).
  - Hydraulic Gradient (i): Derived from water level data across the site (e.g. collected from piezometers). Dimensionless (m/m).
- Transect Area (A): Plume cross-sectional area based on contour boundaries and aquifer thickness. Units: area (e.g. m^2).
- Collection Methods: Uses existing well data; interpolation via software (e.g. kriging); hydraulic data from site records.

5.4.5 Solute Transport Models

- Contaminant Concentrations (C): Initial and boundary conditions from well data (e.g. source zone, downgradient points). Units: mass/volume (e.g. mg/L).
- Hydraulic Parameters:
  - Hydraulic Conductivity (K): Spatially variable or zoned values. Units: length/time (e.g. m/day).
  - Hydraulic Gradient (i): From water level maps or piezometer networks. Units: Dimensionless (m/m).
  - Porosity (n): Effective porosity of the aquifer. Units: Dimensionless.
  - Dispersivity: Longitudinal and transverse values for solute spreading. Units: length (e.g. m).
- Source Characteristics: Mass, location, and release rate of contaminants.

- Boundary Conditions: Heads or fluxes at model edges (e.g. constant head, no-flow boundaries).
- Reaction Parameters (Optional): Biodegradation rates and sorption coefficients if attenuation is modeled.
- Collection Methods: Field data (wells, tests) for calibration; literature or site-specific values for model parameters.

5.4.6 Thermal Tracer Method

- Temperature Measurements:
  - Mixed Water Temperature (T_m): At the point of groundwater-surface water mixing (e.g. streambed, seepage face), measured via probes or Distributed Temperature Sensing. Units: degrees Celsius (°C).
  - Groundwater Temperature (T_g): Stable temperature of discharging groundwater, from wells or upgradient points. Units: °C.
  - Surface Water Temperature (T_s): Temperature of the receiving water body. Units: °C.
- Contaminant Concentration (C): Single or representative value from groundwater or mixed water samples. Units: mass/volume (e.g. mg/L).
- Total Flow Rate (Q_t) (Optional): If measurable (e.g. stream flow), used to scale groundwater discharge. Units: volume/time (e.g. L/s).
- Spatial Context: Location and extent of the mixing zone (e.g. river reach length, depth profile) to define measurement points.
- Collection Methods: Temperature sensors (e.g. thermistors, Distributed Temperature Sensing), groundwater sampling (e.g. wells near discharge), stream gauging (if Qt is needed).

5.4.7 Vapour Flux Estimation

- Isolation (Static) Flux Chamber:
  - Contaminant Mass Collected: Mass of VOCs captured by a passive absorptive sampling tube. Units: mass (e.g. µg).
  - Sampling Duration: Time the chamber is deployed over the surface to allow sufficient VOC capture. Units: time (e.g. hours).
  - Surface Area: Area of the enclosed surface, defined by the chamber's footprint. Units: area (e.g. m^2).
  - GC-MS Analysis Results: Concentrations of specific VOCs from lab analysis to calculate flux. Units: mass/area/time (e.g. µg/m^2/min).
  - Collection Methods: Deployment of static flux chambers on soil, waste, or liquid surfaces; retrieval of sampling tubes; laboratory analysis using GC-MS.
- Dynamic Flux Chamber:
  - Carrier Gas Flow Rate: Volumetric flow rate of clean carrier gas (e.g. nitrogen or zero-air) introduced into the chamber, measured with flow meters. Units: volume/time (e.g. L/min).
  - VOC Concentrations in Exhaust: Concentrations of VOCs in the exhaust gas, sampled in real-time and analyzed via GC-MS. Units: mass/volume (e.g. µg/L).

- Surface Area: Area of the enclosed surface, defined by the chamber's footprint. Units: area (e.g. m^2).
- Collection Methods: Setup of dynamic flux chambers with carrier gas supply and exhaust sampling; continuous or periodic sampling of exhaust gas; laboratory or field-based GC-MS analysis.

5.5 Applications

Mass flux and mass discharge are essential for site characterization, risk assessment, and remediation planning. According to the USEPA (1998a), these metrics serve three primary purposes: evaluating plume attenuation, estimating contaminant release from source areas to inform remedial design, and assessing contaminant loading to receptors. These primary functions underpin the application of mass flux and mass discharge in contaminated site management, as detailed in the Table 5-3. Table 5-4 and Table 5-5 outlines site types where mass flux and mass discharge are either beneficial or not required.

Table 5-3: Applications of Mass Flux and Mass Discharge in Contaminated Site Management

Application	Description	Key Uses
Site Characterization and CSM Development	Supports the development of a CSM by quantifying contaminant distribution and transport.	• Establish baseline mass discharge from source zones. • Identify contaminant hotspots. • Assess mass attenuation rates. • Differentiate multiple sources. • Enhance understanding of contaminant sources, pathways, and receptors at the site.
Plume Delineation	Defines the extent and variability of contaminant distribution.	• Define plume boundaries. • Identify zones of high contaminant mass. • Assess horizontal and vertical plume variability and stability.
Source Zone Characterization	Quantifies contaminant release rates from the source.	• Evaluate contaminant release over time. • Estimate mass loading to groundwater. • Determine persistence of source zone contamination.
Potential Impact and Exposure Evaluation	Assesses risks to receptors by estimating contaminant loads and pathways.	• Quantify contaminant mass reaching receiving environments and/or receptors. • Identify exposure pathways. • Assess risks to sensitive receptors like wells and ecosystems. • Guides risk management decisions by identifying exposure scenarios and pathways.

Application	Description	Key Uses
Natural Attenuation Assessment	Evaluates the reduction of contaminant mass through natural processes.	• Quantify degradation and attenuation rates. • Validate natural attenuation as a remediation approach. • Monitor contaminant mass reduction over time. • Supports decisions on monitored natural attenuation (MNA) as a remediation approach.
Remediation Planning and Design	Informs the design of remediation systems by identifying contaminant hotspots and transport rates.	• Target high-flux zones for remedial system placement. • Optimize remediation designs. • Determine contaminant reduction goals.
Performance Monitoring and Optimization	Tracks remediation effectiveness and helps to refine strategies for optimal contaminant reduction.	• Measure remediation progress. • Identify areas for additional treatment. • Evaluate system efficiency and optimize operation.
Risk Assessment	Estimates contaminant loads reaching sensitive receptors for exposure analysis.	• Provide contaminant flux/discharge data for risk modelling. • Estimate exposure risks to humans and ecological receptors. • Develop site-specific risk thresholds for regulatory compliance and risk-based cleanup criteria.
Vapour Intrusion Risk Assessment	Evaluates health risks from VOCs migrating from contaminated soil or groundwater into indoor air.	• Assess safe building occupancy. • Design mitigation (e.g. vapour barriers, depressurization systems). • Prioritize site remediation.
Contaminant Transport Modelling	Provides input for predictive models of contaminant migration.	• Simulate and/or forecast contaminant migration patterns. • Predict plume behaviour under varying conditions. • Inform long-term management strategies.
Compliance Monitoring	Verifies contaminant discharges meet regulatory requirements.	• Confirm regulatory limits are met. • Validate effectiveness of source control activities or remedial actions. • Monitor compliance with cleanup criteria.
Site Prioritization	Helps rank sites based on contaminant mass and potential risks for resource allocation.	• Rank sites by contamination severity. • Identify high-risk areas for remediation focus. • Allocate resources efficiently based on site risks.

Table 5-4: Relevant Sites for Mass Flux and Mass Discharge Quantification

Type of Site	Reason	Limitations
Relevant Sites		
Sites with groundwater contamination	Useful for quantifying contaminant transport rates and extent of plume contamination in groundwater.	Requires extensive monitoring wells and sampling to accurately map plume dynamics; can be costly and time-intensive.

Type of Site	Reason	Limitations
Relevant Sites		
Hydrocarbon-contaminated sites (e.g. BTEX, PHCs, PAHs)	Effective for assessing the movement of dissolved hydrocarbons (e.g. BTEX, PHCs).	May underestimate contamination in low-permeability zones where hydrocarbons are trapped or sorbed.
Single-source contamination sites (e.g. spills, leaks, releases)	Applicable when contamination originates from a well-defined point source.	Challenging to apply if the source is disperse, not well-characterized or if multiple sources exist.
Sites with measurable plume boundaries (e.g. delineated through monitoring wells or geophysical methods)	Helps delineate the extent and magnitude of a contaminant plume.	Accuracy depends on the density and placement of monitoring points; sparse data can lead to incomplete plume mapping.
Gas plants and compressor stations	Suitable for evaluating the impact of released contaminants (e.g. hydrocarbons, sulphur, amines, sulfolane, glycols, etc.) on groundwater.	Complex site conditions (e.g. variable geology or infrastructure) may complicate accurate flux measurements.
Sites with active remediation strategies (e.g. pump-and-treat or MNA)	Provides baseline data and progress assessment during remediation efforts like pump-and-treat or MNA.	Requires long-term monitoring to assess remediation effectiveness, which can be resource intensive.
Relatively homogeneous aquifers with consistent permeability and flow characteristics	Better suited for aquifers with consistent permeability and flow characteristics.	Potential oversimplification of contaminant transport dynamics, as it may fail to detect subtle localized variations in aquifer properties or unexpected changes in flow due to external influences like nearby pumping wells.
Sites with clear regulatory drivers for plume management and risk assessment	Often required to meet regulatory needs for plume management and risk assessment.	May require additional data collection to meet specific regulatory standards, increasing project complexity.

Table 5-5: Unsuitable Sites for Mass Flux and Mass Discharge Quantification

Type of Site	Reason
Sites with highly heterogeneous geology (e.g. varying soil layers, fractures, or karst formations)	Challenging due to variability in flow and contaminant transport pathways making a meaningful assessment labour intensive.
Site with multiple sources of contamination (e.g. industrial complexes with multiple spill points or diffuse pollution sources)	Difficult to isolate contributions from different sources for accurate quantification of mass flux.
Sites dominated by NAPLs	Less effective if the contaminant is primarily in a NAPL phase with limited dissolution.
Sites with negligible groundwater flow (e.g. areas with low hydraulic conductivity or stagnant water conditions)	Not applicable if groundwater movement is insufficient to transport contaminants.
Complex urban environments (e.g. cities with underground infrastructure, mixed land use, and variable subsurface conditions)	High variability in subsurface conditions can reduce accuracy and practicality, particularly where preferential pathways materially affect flow.
Sites without defined monitoring points (e.g. locations lacking established wells or sampling stations)	Requires clear plume boundaries and monitoring wells for accurate calculations.

Type of Site	Reason
Sites with limited data availability (e.g. insufficient historical records or sparse sampling data)	Ineffective without sufficient hydrogeological data (e.g. detailed aquifer properties, flow rates) and contaminant concentration data (e.g. regular measurements across the plume).

5.6 Relationship to Alberta Policy

5.6.1 Current Status

The use of mass flux and mass discharge of contaminants as a decision-making tool in contaminated sites investigation, remediation and risk assessment is currently recognized within current Alberta policy as summarized below.

- Current ESA guidance allows for mass flux to be utilized to support CSM development (AEPA 2024c).
- The standard Tier 1 and Tier 2 models for groundwater transport include mass flux calculations to estimate groundwater to surface water transport (AEPA 2023; 2024a; 2024b). Alternative models are also permitted within risk assessment with appropriate consultation (AEP 2023).
- While not explicitly documented within Alberta written policy and guidance documents, mass flux and mass discharge has precedent of being an acceptable line of evidence to inform site-specific risk assessment.
- While not explicitly documented within Alberta written policy and guidance documents, mass flux may be incorporated in complex fate and transport models. Complex fate and transport models are documented as an acceptable line of evidence to support risk assessment and long-term risk management (AEP 2023).

5.6.2 Gaps in Alberta Policy and Opportunities for Improvement

There are gaps in Alberta's written policy and guidance about how to calculate mass flux and mass discharge, which methods / guidance documents AEPA and AER consider acceptable, limitations on when mass flux and mass discharge calculations can be used; what site-specific measurements are required to validate mass flux and mass discharge calculations and what model input parameters are acceptable. To address these gaps, it would be beneficial to provide formal written policy and/or guidance that describes:

- When AEPA / AER consider mass flux and/or mass discharge to be an acceptable metric to describe contamination within a CSM;
- What site-specific conditions preclude the calculation of mass flux and/or mass discharge to describe contamination within a CSM;
- What specific methods/guidance AEPA / AER considers acceptable when calculating mass flux / mass discharge;
- What site-specific conditions preclude the use of mass flux and/or mass discharge calculations in support of site investigation, remediation and/or risk assessment;
- What input parameters are acceptable in mass flux and/or mass discharge calculations including, as appropriate:
  - Use of default versus site-specific parameters;

- When site-specific data must be collected and what methods will be considered applicable; and
- How to approach situations where site-specific information is unavailable or is impracticable to collect/measure.

Providing written policy and/or guidance on the methods and key assumptions that are acceptable to AEPA and AER for estimating total mass would provide consistency in these evaluations, limit rework and minimize potential for both submission returns and SIRs.

5.7 Costing

The following table presents a cost estimate for quantifying mass flux and mass discharge using various methods, including transect methods, well capture / pump tests, passive flux meters, isocontours, and solute transport models for a standard oil and gas lease in Alberta (see Section 1.3.1 for definition and assumptions).

Table 5-6: Cost Estimate for Mass Flux and Mass Discharge Quantification Methods for a Standard Oil and Gas Lease

Approach	Description	Data Required	Purpose	Strengths	Challenges	Primary Uses
Transect Methods	Estimates contaminant mass flux along a cross-sectional transect of the plume by installing monitoring points and collecting concentration and flow data.	Groundwater contaminant concentrations. Groundwater flow velocities. Transect layout (spacing and number of monitoring points).	Evaluate spatial distribution of flux. Identify high-flux zones for targeted remediation. Refine CSM.	High spatial resolution. Identifies high-flux zones.	Requires high-resolution characterization data. Potential for interpolation errors if the sampling density or spatial variability is not adequately captured. Cost-intensive for sampling and analysis.	Accurately map and quantify the total contaminant mass discharging into a receiving environment using high spatial resolution data. Characterizing plumes, identifying remediation zones, and estimating natural attenuation.
Well Capture/Pump Tests	Groundwater is pumped from one or more wells to measure total contaminant mass discharge and groundwater flow directly.	Total volume of groundwater extracted. Contaminant concentrations in the extracted water. Well placement and pumping rates must be such that the full extent of the plume is captured.	Directly measure total contaminant mass discharge at a specific location or across a specific area. Confirm remediation effectiveness by monitoring changes in mass discharge over time.	Reduces interpolation error compared to transect methods. High certainty of capturing contaminant flux at the selected location. Effective for compliance monitoring and plume characterization.	Requires significant infrastructure, including wells and pumps (e.g. larger diameter wells are useful for higher pumping rates or longer-term extraction). Generates large volumes of water that may require treatment and disposal. Does not provide spatial distribution data within the plume and is limited by the effectiveness of well placement and selected pumping rates.	Provides for direct measurement of total mass discharge at specific locations. Assessing total mass discharge, evaluating pump-and-treat systems, and verifying remediation progress.
Passive Flux Meters	Directly measures contaminant and water flux over time using passive flux meters that are placed in wells for a set duration. The devices absorb contaminants and measures the volume of water passing through the well. Data collected are analysed to calculate both contaminant and groundwater flux.	Device deployment data, including placement and duration of measurements. Absorbed contaminant mass and water flux (rate of groundwater flow through a unit area perpendicular to the flow direction) measurements.	Measure localized contaminant transport rates. Provide continuous data over the deployment period.	Simple deployment and retrieval. Disturbance to the site is minimal and no purge water is generated. Reduces the need for frequent sampling or monitoring.	Limited to the area immediately surrounding the well. May require site-specific calibration to account for varying conditions. Does not provide high spatial resolution data across the plume unless deployed in multiple locations.	Quick, low-disturbance approach for localized measurements; long-term, passive monitoring. Monitoring post-remediation fluxes and tracks mass reduction pre/post-treatment.
Transects Based on Isocontours	Estimates mass discharge indirectly by multiplying groundwater flow rates and contaminant concentrations collected from monitoring wells or isocontours.	Groundwater flow rates and hydraulic conductivity data. Contaminant concentrations from monitoring wells or isocontour maps.	Provides a cost-effective means to estimate mass discharge. Useful for sites with extensive existing monitoring data.	Leverages existing data, reducing the need for new fieldwork. Useful for initial estimates of mass discharge. Cost-effective.	Highly dependent on the quality and spatial resolution of input data. May underestimate discharge if high-flux zones are not adequately sampled / characterized. Less accurate than other approaches.	Provides cost-effective estimates of mass discharge where detailed field work is not needed. Preliminary estimates of mass discharge; supporting plume stability analysis.
Solute Transport Models	Numerical solute transport models use input data such as groundwater flow rates, contaminant concentrations, and site-specific hydrogeological parameters to simulate contaminant transport and calculate mass discharge.	Contaminant concentration data. Groundwater flow rates and hydraulic conductivity values. Site-specific parameters, such as porosity and dispersion coefficients.	Predict future plume behaviour under different scenarios. Evaluate the effectiveness of natural attenuation and remediation strategies.	Flexible and capable of simulating complex systems. Useful for assessing long-term plume behaviour and risks.	Requires extensive, high-quality input data. Complex to set up and calibrate, especially for heterogeneous aquifers. Results are model-dependent and may not fully reflect site-specific conditions.	Provides long-term predictions and input into development of remediation strategies.
Thermal Tracer Method	Uses temperature mixing to estimate groundwater discharge, paired with measured concentration.	Temperatures (groundwater, surface water, point of groundwater and surface water mixing), concentration, total flow (optional), location and extent of mixing zone.	Estimate bulk mass discharge at discharge interfaces (e.g. streams).	Non-invasive; leverages natural thermal signals; cost-effective for large areas.	Requires thermal contrast; limited to mixing zones; sensitive to thermal noise.	Groundwater contaminant loading to surface water (e.g. rivers, lakes).
Isolation (Static) Flux Chamber	Encloses a surface area with a passive absorptive sampling tube (e.g. containing activated carbon or polymer resins) to capture VOCs via molecular diffusion over a set period. VOC mass is analysed using GC-MS to calculate flux.	VOC mass collected, sampling duration, surface area, GC-MS analysis results.	Quantify diffusive VOC emissions from soil, waste, or liquid surfaces to assess contamination and vapour intrusion risks.	Cost-effective, minimal equipment, no power required, suitable for long-term monitoring.	Limited to diffusive flux, slower data collection, less precise for variable emissions.	Long-term monitoring of stable, diffusive VOC emissions at contaminated sites, especially in remote areas.

Approach	Description	Data Required	Purpose	Strengths	Challenges	Primary Uses
Dynamic Flux Chamber	Encloses a surface area and introduces a continuous flow of clean carrier gas (e.g. nitrogen or zero-air) to mix with emitted vapours. Exhaust gas is sampled in real-time and analysed via GC-MS to calculate flux (µg/m²/min).	Carrier gas flow rate, VOC concentrations in exhaust, surface area, GC-MS analysis results.	Measure real-time VOC emissions to assess transient or variable sources and support immediate risk evaluations.	High precision, real-time data, effective for variable emissions, adaptable to different surfaces.	Requires power, complex setup, higher cost, sensitive to carrier gas quality and flow consistency.	Real-time assessment of VOC emissions, particularly for dynamic or heterogeneous sources at contaminated sites.

These estimates are approximate and can vary based on site-specific conditions, regional labor rates, and the complexity of the contamination. Costs will generally be reduced if data are collected concurrently with CSM development and/or execution of other field programs.

5.8 Summary

Mass flux and mass discharge methods quantify contaminant movement in groundwater or soil vapour, with mass flux measuring the rate through a specific area and mass discharge calculating the total mass across a control plane, relying on data like contaminant concentrations, hydraulic conductivity, and groundwater flow velocities. These methods necessitate detailed data gathering, utilizing tools like monitoring wells, pumping tests, or passive flux meters to effectively track variations. Consequently, the approaches can become cost-intensive, requiring sophisticated monitoring systems, advanced sampling methods, and multiple assessments to address the spatial and temporal changes in contaminant plumes. In contaminated site management, they improve site characterization, risk assessment, and remediation planning by identifying source strengths, plume behaviours, and treatment zones, supporting regulatory compliance and more effective decision-making.

6. Mass Transfer Assessment

6.1 Description

Mass transfer refers to the movement of particles or chemical species from areas of higher concentration to lower concentration, driven by factors such as concentration gradients, mechanical forces, thermal effects, or redox conditions (USEPA 2010). Redox cycling and acidification (e.g. sulfide mineral oxidation [SMO], acid mine drainage [AMD], and neutral mine drainage [NMD]) play a significant role in mass transfer within soil, water, and air systems.(Mass transfer can occur within a single medium (e.g. soil, water, or air) or across environmental media (e.g. from soil to groundwater or from groundwater to surface water) via processes like diffusion, advection, or pressure-driven flow. Understanding mass transfer is crucial for assessing contaminant fate and transport at contaminated sites, as it helps explain how pollutants spread, transform, and interact within and between different media (Essaid et al. 2015).

A mass transfer assessment quantifies the rate at which contaminants move, providing essential information for risk assessment, remediation planning, and long-term site management. Several factors influence the rate and efficiency of mass transfer in contaminated environments, including:

- Concentration Gradient: The more pronounced the concentration gradient, the stronger the driving force for mass transfer, accelerating the movement of contaminants from more contaminated to cleaner zones.
- Fluid Properties: The viscosity, density, vapour pressure, solubility and temperature of the involved fluids significantly impact mass transfer rates. Low-viscosity fluids allow faster contaminant movement, while density differences can lead to stratification and affect transport pathways. Vapour pressure dictates the tendency of contaminants to volatilize, with higher values increasing mass transfer to the gas phase. Solubility governs how readily contaminants dissolve into or move between fluids, affecting their mobility. Temperature influences molecular kinetic energy, with higher temperatures enhancing diffusion rates and improving overall mass transfer efficiency.
- Surface Area: A larger interface surface area between environmental phases (e.g. soil-water, water-air) enhances mass transfer potential. For example, contaminants volatilize more easily from groundwater when exposed to a larger water-air interface.
- Tortuosity: The complexity of contaminant pathways through porous materials like soil, sediment, or compacted waste impacts mass transfer. In highly tortuous materials, contaminants must travel longer, winding paths, which slows diffusion by extending the effective distance they must cover (USEPA 2010; CCME 2016).

In contaminated sites, the transport of contaminants is governed by several mass transfer processes, including advection, diffusion, dispersion, and volatilization (CCME 2016). These processes govern the movement of contaminants between phases (e.g. from water to air) or within a single phase (e.g. groundwater). Advection involves the bulk movement of contaminants carried by fluid flow, such as groundwater moving through porous media, and typically dominates in high-permeability zones or systems with significant hydraulic gradients. Diffusion, driven by concentration gradients, plays a crucial role in low-permeability zones or stagnant conditions, such as within fine-grained soils. Dispersion spreads contaminants as a result of variations in flow

velocity and direction within the subsurface, enhancing the extent of contaminant plumes. Volatilization transfers contaminants from liquid or solid phases into the vapour phase, contributing to risks like soil vapour intrusion into indoor air (CCME 2016).

Understanding the interplay of these processes is essential for accurately predicting contaminant behaviour, assessing exposure risks, and selecting effective remediation strategies. For example, while concentration-based assessments may indicate regulatory compliance in groundwater, mass transfer analysis incorporating diffusion, dispersion, and volatilization can reveal ongoing contaminant release from low-permeability zones or soil vapour migration into buildings (CCME 2016). Such insights inform the design and optimization of remediation technologies, such as soil vapour extraction for volatile contaminants, pump-and-treat systems for advective transport, or in-situ chemical oxidation for diffusion-limited zones.

Mass transfer assessments are particularly valuable in complex subsurface environments, where variations in soil structure, fluid properties, and contaminant phases can significantly influence transport pathways (CCME 2016). By incorporating these principles, environmental professionals can more accurately predict contaminant behaviour and refine remediation approaches providing for long-term protection of both human health and the environment. Furthermore, such assessments are key to identifying secondary contamination pathways, such as vapour intrusion from groundwater plumes into indoor spaces, supporting comprehensive site management and risk mitigation.

6.2 Media Considered

A mass transfer assessment evaluates contaminant movement within and between environmental media, requiring consideration of multiple media types to characterize transport pathways, transformation processes, and exposure risks. The primary media assessed in mass transfer evaluations include soil, groundwater, surface water, sediment, soil vapour and air, each contributing to the overall fate and transport of contaminants in different ways.

- **Soil:** Soil serves as a primary medium for contaminant retention and transport, influencing mass transfer through adsorption, desorption, diffusion, and advection. Contaminants in soil can migrate vertically or laterally due to water infiltration, capillary action, or volatilization. The nature of soil—such as grain size, porosity, and organic matter content—affects mass transfer rates. Fine-grained soils (e.g. clays) exhibit lower permeability and increased tortuosity, limiting advective transport but enhancing diffusion-controlled processes. Coarse-grained soils (e.g. sands and gravels) facilitate advection-driven mass transfer, often leading to rapid contaminant migration (CCME 2016).
- **Groundwater:** Groundwater acts as a primary transport medium for dissolved contaminants, facilitating advection, dispersion, and diffusion. Groundwater flow velocity, hydraulic gradient, and aquifer properties (e.g. permeability, porosity) govern mass transfer rates. Contaminants can migrate through groundwater plumes, undergoing dilution, chemical transformation, or retardation due to sorption onto aquifer materials. Mass transfer in groundwater is essential for understanding contaminant persistence, plume stability, and remediation feasibility (USEPA 2010).
- **Surface Water:** Surface water systems (e.g. streams, rivers, lakes, and wetlands) contribute to contaminant transport through advection, dispersion, sediment-water interactions, and

volatilization. Hydrodynamic conditions, including flow velocity, turbulence, and temperature, influence contaminant mixing and distribution. The exchange between groundwater and surface water, driven by hydraulic gradients and permeability contrasts, is critical for assessing mass transfer pathways and contaminant fate (Essaid et al. 2015).

- **Sediment:** Sediments act as both sinks and secondary sources of contaminants, influencing mass transfer through sorption-desorption equilibria, diffusion, and bioturbation. Fine-grained sediments with high organic carbon content can adsorb hydrophobic contaminants, reducing bioavailability but creating potential long-term contamination reservoirs. Diffusion-driven mass transfer between sediment porewater and overlying water can lead to contaminant release, particularly under changing redox conditions (CCME 2016).
- **Soil Vapour:** Soil vapour acts as a key transport medium for volatile contaminants, influencing exposure risks through vapour intrusion into buildings and ambient air emissions. Mass transfer processes governing soil vapour include diffusion, advection, and volatilization from contaminated soil or groundwater. The permeability of the subsurface, presence of preferential pathways (e.g. utility corridors, fractures), and barometric pressure changes can affect vapour migration. Assessing soil vapour is critical for evaluating indoor air exposure risks and designing vapour mitigation measures (USEPA 2015; USEPA 2021b).
- **Air:** The atmosphere plays a role in mass transfer through volatilization, particulate transport, and gas-phase diffusion. Contaminants with high vapour pressures (e.g. VOCs) can transfer from soil or water to air, contributing to soil vapour intrusion and inhalation exposure risks. Wind speed, temperature, and atmospheric stability influence contaminant dispersion and transport distances. Mass transfer assessments consider air-phase contamination to evaluate potential exposure pathways and inform vapour mitigation strategies (CCME 2016).

6.3 Approach

A mass transfer assessment involves the systematic process of evaluating the transport of a substance from an area of higher concentration to an area of lower concentration, including from one phase to another (Fiveable 2024). The goal is to understand the fate and transport of pollutants and assess their potential impact on human health and the environment. Depending on the system and context, mass transfer can be quantified using various methods. Below are the key aspects of calculating or measuring mass transfer.

Fick's Laws of Diffusion

Fick's Laws of Diffusion are key principles in mass transfer, as they describe how particles move from regions of higher concentration to regions of lower concentration, establishing a relationship between the diffusion flux and the concentration gradient. Mass transfer can be quantified using Fick's First Law (Steady-State Diffusion), which describes the diffusive flux of a substance as it relates to a concentration gradient (CCME 2016; Fiveable 2024). For a one-dimensional case, the diffusive flux can be described by:

$$J = -D\frac{dC}{dx} \qquad \textbf{Equation 6-1}$$

where:

J = diffusive flux (mass per unit area per unit time; mass flux; e.g. kg/m²·s)

D = diffusion coefficient (a measure of how easily a substance diffuses, with negative sign indicating that diffusion occurs in the direction opposite to the concentration gradient; e.g. m^2/s)

$\frac{dC}{dx}$ = concentration gradient (the change in concentration per unit distance; e.g. kg/m^3 per meter)

Accurately solving steady-state diffusion problems in one-dimensional systems requires details on boundary conditions to determine the concentration profile and diffusive flux. These conditions include fixed concentrations, no-flux conditions at impermeable boundaries, and continuity of concentrations and flux at interfaces (Willson et al. 2000; Asano 2006; CCME 2016).

When the concentration of a substance changes over time, the use of Fick's Second Law (Transient Diffusion) is required. This law describes the changes in concentration of a substance over time due to diffusion, and is described by:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad \textbf{Equation 6-2}$$

where:

$\frac{\partial C}{\partial t}$ = rate of concentration change over time at a fixed point in space, driven by diffusion

C = concentration of the substance

t = time

D = diffusion coefficient ((which determines the rate at which diffusion spreads concentration changes in a medium))

x = spatial coordinate

$\frac{\partial^2 C}{\partial x^2}$ = the second spatial derivative of concentration, indicating how the concentration gradient is changing along the spatial coordinate (Fiveable 2024).

In multi-dimensional systems, diffusion occurs across two or three spatial dimensions, requiring an extension of Fick's laws to account for additional spatial derivatives. Analysing diffusion in multi-dimensional systems involves solving Fick's second law with appropriate initial and boundary conditions, which adds complexity compared to one-dimensional cases and often requires software solutions to support the computation (Fiveable 2024).

Mass Transfer Coefficient

The mass transfer coefficient (*k*) relates the mass transfer rate to the concentration difference across a boundary layer, such as between a surface and the bulk fluid. It quantifies how effectively a substance is transferred between phases (e.g. liquid to gas) or through a medium. Mass transfer coefficients are particularly relevant in convective mass transfer processes, where transport of a substance occurs through the combined effects of bulk fluid motion (advection) and molecular diffusion, as well as in systems involving diffusion across boundary layers. The mass

transfer coefficient, once determined from empirical data or system-specific measurements, enables the calculation of the mass transfer rate (M) in the context of contaminated sites—such as predicting the spread of pollutants from soil to groundwater or the volatilization of contaminants into the air—by relating it to the concentration driving force and transfer area, providing a practical tool to assess and optimize remediation strategies where diffusion alone (e.g. Fick's Law) is insufficient to describe the process.

Mathematically, the mass transfer coefficient is expressed as:

$$k = \frac{M}{A * \Delta C_A} \qquad \textbf{Equation 6-3}$$

where:

k = mass transfer coefficient (e.g. m/s)

M = mass transfer rate (amount of substance transferred per unit time, e.g. kg/s or mol/s)

A = mass transfer area (e.g. m^2)

ΔC_A = concentration difference of substance in the bulk phase and at the interface or surface (e.g. kg/m^3 or mol/m^3; Seader and Earnest 1998).

This equation highlights that the mass transfer rate (M) depends on the mass transfer area, the concentration gradient, and the efficiency of mass transfer as described by the coefficient (k). Unlike Fick's Law, which provides a diffusive flux based on a gradient within a medium, the mass transfer coefficient simplifies complex convective processes across interfaces at contaminated sites, often derived from empirical correlations or experimental data, making it a practical tool for modelling contaminant transport and evaluating cleanup effectiveness.

Empirical Models

At contaminated sites, mass transfer rates are often estimated using empirical correlations that relate mass transfer coefficients to dimensionless numbers, such as the Reynolds number, Schmidt number, and site-specific geometries (Asano 2006). These correlations are valuable for predicting mass transfer in complex environments like fractured rock or engineered remediation systems, where direct measurement may be difficult. For instance, the Sieder-Tate equation is used to estimate mass transfer in groundwater flow, while Onda and Shulman correlations are applied to packed beds and soil columns (Tosun 2007). However, adapting these flow equations from controlled systems (e.g. pipes or columns) to heterogeneous environmental systems requires careful consideration of boundary conditions. Defining appropriate boundary conditions involves identifying analogous interfaces (e.g. replacing pipe walls with impermeable layers), incorporating site-specific hydraulic properties (e.g. permeability, porosity), setting concentration boundaries using field data (e.g. contaminant levels at sources and interfaces), accounting for temporal and spatial variability (e.g. precipitation effects), and validating model predictions with field measurements or numerical simulations. This ensures the empirical models reflect the

complex conditions of contaminated sites, allowing them to assess contaminant movement through media, guide the design of remediation technologies such as soil vapour extraction or pump-and-treat systems, and improve predictions of treatment efficiency and contaminant behaviour.

The following table provides definitions of concepts related to mass transfer empirical models.

Table 6-1: Concepts used in Estimating Mass Transfer

Term	Definition	Application to Contaminated Sites
Reynolds Number (Re)	A dimensionless quantity used to predict the flow regime (laminar or turbulent) by comparing inertial forces to viscous forces (Fiveable 2024).	Used to characterize groundwater flow through porous media (e.g. aquifers) or air flow in soil vapour extraction systems, helping predict whether flow is laminar or turbulent, which affects contaminant transport.
Schmidt Number (Sc)	A dimensionless ratio of kinematic viscosity to mass diffusivity, expressing the relative importance of momentum diffusion to molecular diffusion in a fluid (Fiveable 2024).	Applied in modelling the diffusion of contaminants in groundwater or air, such as VOCs in soil gas, to understand how quickly contaminants spread relative to fluid motion.
Sieder-Tate Equation	An empirical formula used to estimate mass transfer coefficients in laminar flow in pipes, considering temperature effects (Fiveable 2024).	Useful in designing remediation systems like pump-and-treat, where contaminants are extracted through pipes, accounting for temperature effects on mass transfer in groundwater flow.
Onda Correlations	Empirical correlations used to estimate mass transfer coefficients in packed beds, based on system geometry and flow conditions (Fiveable 2024).	Relevant for air stripping or soil vapour extraction in packed bed reactors, where contaminants are removed from groundwater or soil, relying on geometry and flow to optimize mass transfer.
Shulman Correlations	Empirical models for calculating mass transfer coefficients in packed beds or porous media, considering flow configurations and system characteristics (Fiveable 2024).	Applied in bioremediation or filtration systems for contaminated sites, where mass transfer in packed beds (e.g. activated carbon filters) is critical for removing pollutants from water or air.

Experimental Methods

Experimental evaluation of mass transfer relies primarily on laboratory-based approaches such as batch experiments and column studies, with results later integrated into site-specific mathematical models, while field studies provide in situ data to validate these models and account for non-ideal mass transfer processes in real-world settings. Mass transfer can be evaluated through a variety of experimental setups designed for specific conditions and objectives. Results from these experiments are then integrated into site-specific mathematical models to account for non-ideal mass transfer processes. Examples of these processes include the effects of sorption, biodegradation, and water table fluctuations; spatial and temporal variations in contaminant composition; and spatial and temporal variations in saturation. Collectively these variables impact the dissolution and long-term transport of dissolved plumes in the subsurface (Vasudevan et al. 2016).

Batch experiments, a commonly used laboratory technique, are used to measure changes in contaminant concentrations over time, allowing researchers to calculate removal rates and determine partitioning coefficients. In these experiments, a known quantity of contaminant is

added to a medium—typically an aqueous solution or a soil-water slurry—and samples are taken at regular time intervals to determine concentration changes, providing insights into the kinetics and thermodynamics of the mass transfer process (Sale and McWhorter 2001).

Column studies are used to assess mass transfer characteristics by simulating the transport of substances between phases under controlled laboratory conditions (Ilea et al. 2020). By varying factors such as fluid velocity, packing material, and chemical composition, these studies quantify key parameters like mass transfer coefficients, effective mass transfer areas, and phase interactions. For example, in a three-phase fluidized column operating as an open system with continuous counter-current flow of gas and liquid, the presence of gas, liquid, and solid phases allows researchers to evaluate how turbulence, surface area, and physical mixing enhance mass transfer rates compared to traditional packed beds (Ilea et al. 2020).

Field studies represent a transition from laboratory to in situ monitoring to validate laboratory findings and assess mass transfer under natural conditions. Field studies can include the following:

- **Monitoring Well Installation:** Establishing monitoring wells at strategic locations enables the collection of groundwater samples to analyse contaminant concentrations over time. This approach provides insights into contaminant distribution and migration patterns (CCME 2016). For groundwater-surface water interactions, nested wells and piezometers placed at varying depths help assess vertical hydraulic gradients and exchange processes. Isotopic and geochemical tracers can further delineate groundwater contributions to surface water and contaminant fluxes. Note that monitoring wells may have limitations in resolving localized variations in contaminant concentrations and can be influenced by heterogeneities in subsurface conditions.
- **Soil Vapour Extraction (SVE):** SVE involves extracting volatile contaminants from the soil by applying a vacuum, facilitating the removal of contaminants from the vadose zone and potentially enhancing volatilization from the capillary fringe. SVE measures the concentration and flow rate of the off-gas, calculates the mass removed over time, and uses this data to assess kinetics and partitioning. However, SVE effectiveness depends on soil permeability, organic carbon content (f_{oc}), and site-specific partitioning characteristics. This method is particularly effective for sites with high vapour-phase contaminant concentrations (CCME 2016). For cross-media transport analysis, SVE field studies can quantify volatilization rates and the potential for contaminant migration into the atmosphere, influencing air quality assessments.
- **Vapour Probe Installation:** Installing vapour probes or vapour wells enables the collection of soil gas samples to assess vapour-phase contaminant concentrations, aiding in vapour intrusion assessments. When integrated with groundwater monitoring, vapour sampling can help evaluate the role of fluctuating groundwater tables in enhancing VOC emissions. Indoor air sampling can complement these measurements to evaluate potential exposure risks.
- **Porewater and Sediment Sampling:** Porewater sampling and sediment coring provide direct measurements of contaminant concentrations in low-permeability zones and depositional environments, which can be essential for natural attenuation studies by tracking biogeochemical indicators such as redox conditions, microbial activity, and degradation byproducts. In groundwater-surface water interaction studies, porewater samples collected along hyporheic zones can reveal contaminant fluxes and attenuation mechanisms at the interface.

- **Contaminant Elution Tests (CETs):** Induced-gradient CETs assess mass-removal behaviour and characterize the impact of mass-transfer and attenuation processes on contaminant transport. These tests help measure contaminant mass discharge and evaluate remediation effectiveness (Brusseau et al. 2006). For natural attenuation assessments, CETs can quantify the desorption-limited release of contaminants and inform long-term stability predictions. Limitations include potential scale effects and challenges in extrapolating results to field-scale conditions.
- **Tracer Tests:** Injecting non-reactive tracers, such as bromide, chloride, and deuterium-labeled water, with similar physico-chemical characteristics as target compounds into the subsurface allows for the tracking of groundwater flow and contaminant transport dynamics. Tracer tests help delineate flow paths and estimate transport parameters but do not directly quantify contaminant mass transfer rates (DeSimone et al. 1997; Willson et al. 2000). For groundwater-surface water interaction studies, temperature and isotopic tracers can track exchange rates, while reactive tracers can assess biodegradation and sorption processes. These tests are often limited by the representativeness of the tracers used and may not fully capture complex multi-phase transport processes.

- **Geophysical Surveys:** Techniques such as electrical resistivity tomography and ground-penetrating radar provide spatial imaging of subsurface structures, aiding in the identification of salinity plumes and heterogeneities. For cross-media transport analysis, these methods can detect zones of groundwater seepage into surface water, identify preferential flow paths, and map buried contaminant plumes. These methods can help identify stratigraphic controls on contaminant transport but are generally limited in detecting hydrocarbon contamination and resolving fine-scale permeability variations (Contaminated Site Clean-Up Information (CLU-IN n.d.).

- **Field-Based Mass Transfer Characterization:** Assessing site-specific properties such as f_{oc}, permeability, porosity, and contaminant partitioning through field investigations, including leachability studies and tools like lysimeters and kinetic cells, provides direct insights into mass transfer processes and informs remediation strategies. For natural attenuation studies, long-term monitoring of degradation intermediates, electron acceptors, and microbial community structure can help evaluate intrinsic remediation potential. Field studies capture the complex interactions occurring under natural conditions, providing valuable data to refine laboratory models and assess the effectiveness of remediation strategies in environmental applications.

6.4 Data Requirements

The following data requirements are specific to mass transfer assessment, which extend beyond baseline CSM data, to quantify the rates and processes of contaminant movement within and across environmental media, enhancing predictions of fate, transport, and remediation effectiveness.

- Quantified Physical Framework for Phase Interfaces:
  - Soil properties: grain size, porosity, permeability, organic carbon content.
  - Hydrogeological data: hydraulic conductivity.
  - Geospatial data: topography, stratigraphy, subsurface heterogeneity.
  - Fluid properties: density, viscosity, solubility, interfacial tension.

- Direct measurements: geophysical surveys.
- Environmental conditions: pressure.

- Diffusion Paths:
  - Assessment of tortuosity in soil or sediment via core sample analysis to refine site-specific diffusion pathways.
- Concentration Gradient Data:
  - Contaminant concentrations at source and receptor points, vertical and horizontal profiles, interface transition concentrations, measurements across key interfaces (water-air, sediment-water, or soil-gas), and phase-specific concentrations: dissolved, vapour, or particulate-bound.
- Mass Transfer Coefficients:
  - Derivation of site-specific coefficients (k) for processes such as volatilization and interphase mass transfer (e.g. gas-liquid or soil-water exchange) using empirical correlations or field measurements.
- Boundary Conditions:
  - Media properties: moisture content, water table depth.
  - Hydraulic gradients or flow rates, atmospheric conditions, seasonal variations, and supplemental data from additional wells to establish no-flux zones or flow boundaries at the site's spatial and temporal limits.
- Process-Specific Field Data:
  - Advection (e.g. groundwater velocities and flow direction), dispersion (e.g. plume spread), volatilization (e.g. vapour flux), sorption/desorption rates (e.g. partition coefficients from soil or sediment), dissolution rates (e.g. from NAPLs and other residual phases into groundwater), biodegradation rates (e.g. microbial degradation kinetics), phase partitioning behaviour (e.g. Henry's Law constants for gas-liquid interfaces).
- Redox and Biogeochemical Data:
  - Redox conditions, pH, microbial activity (e.g. via molecular probes), dissolved oxygen levels, electron acceptor concentrations (e.g. nitrate, sulphate, or iron), total organic carbon availability, and specific metabolite or daughter product concentrations (e.g. from chlorinated solvent degradation).
- Temporal and Spatial Variability:
  - Monitoring of flow rates, temperature, turbulence characteristics, and seasonal flow or temperature fluctuations at an appropriate spatial and temporal resolution to capture variability in mass transfer processes.
- Experimental Validation Data:
  - Laboratory or field experiments (e.g. batch tests, column studies, flow-through reactor tests, contaminant elution tests, tracer studies) to generate kinetic and partitioning data and calibrate mass transfer models.

6.5 Applications

Mass Transfer Assessments are widely used in contaminated site management to support decision-making for remediation strategies, risk assessments, and regulatory compliance. Table

6-2 outlines key applications of Mass Transfer Assessments, their descriptions, and the specific uses that guide effective site management and remediation. Table 6-3 and Table 6-4 outlines site types where mass transfer is either beneficial or not required.

Table 6-2: Applications of Mass Transfer Assessments in Contaminated Site Management

Application	Description	Key Uses
Vapour Intrusion Assessment	Evaluates the movement of volatile contaminants (e.g. VOCs) from soil and/or groundwater into indoor air.	• Identify buildings at risk of vapour intrusion. • Design mitigation systems (e.g. sub-slab depressurization). • Assess risks to indoor air quality.
Leachate Migration Analysis	Quantifies the mass transfer of leachate from contaminated soil or waste sources into groundwater, surface water and sediments.	• Identify high-risk areas for groundwater contamination. • Optimize monitoring well placement. • Design containment systems (e.g. liners or caps). • Acidification impact assessment.
Groundwater-Surface Water Interaction	Assesses the transport of contaminants from groundwater to adjacent surface water bodies and their respective sediments.	• Predict contaminant flux to surface water and attenuation in sediments. • Design protective barriers (e.g. sediment traps and permeable reactive barriers [PRBs]). • Inform ecological risk assessments for aquatic habitats.
Natural Attenuation Studies	Aids in estimating the rates of biodegradation, volatilization, dispersion, adsorption, dilution or other natural processes reducing contaminant mass.	• Support MNA as a remediation strategy. • Evaluate the effectiveness of natural degradation processes. • Inform long-term management plans.
Remediation System Design	Estimates contaminant removal rates during remediation (e.g. SVE, pump-and-treat).	• Predict the efficiency of remediation techniques. • Optimize remediation system parameters (e.g. flow rates, extraction points). • Reduce cleanup time and costs.
Cross-Media Transport Analysis	Evaluates contaminant transfer between environmental media (i.e. soil, sediments, bedrock, water, vapour, and air environments).	• Identify dominant transport pathways. • Prioritize remediation efforts based on significant migration routes. • Assess risks to multiple environmental media.
Flux Evaluation	Quantitative analysis of the rate at which contaminants move across a boundary or between environmental media.	• Predict migration distances of contaminants. • Inform risk-based corrective actions. • Assess potential impacts to receptors.
Source Zone Delineation	Assesses the movement of contaminants away from a defined source area.	• Map contaminant plume boundaries. • Evaluate source control options. • Design focused remediation strategies.
Heavy Metal Transport Assessment	Models the movement of heavy metals in soil and water.	• Predict metal leaching potential. • Assess risks to receiving waterbody and drinking water supplies. • Design sediment or groundwater remediation or containment systems.

Application	Description	Key Uses
Surface Water Protection	Evaluates the movement of contaminants into receiving waterbodies (e.g. streams, rivers, lakes and wetlands).	• Develop strategies to limit downstream contamination. • Inform regulatory compliance for surface water quality. • Assess impacts on aquatic ecosystems.

Table 6-3: Relevant Sites for Mass Transfer Assessment

Type of Site	Reason	Limitations
Site contaminated with petroleum hydrocarbon (e.g. oil refineries, gas stations, gas plants, well sites, compressor station)	Mass transfer is essential for evaluating volatilization, dissolution, and diffusion of hydrocarbons, especially BTEX and Light Non-Aqueous Phase Liquids (LNAPLs).	The presence of impermeable subsurface barriers or low-permeability layers may restrict the movement and mass transfer of hydrocarbons, leading to uneven contaminant distribution and remediation challenges.
Chlorinated solvent sites (e.g. industrial dry-cleaning facilities, maintenance facilities)	Mass transfer methods are critical for assessing DNAPL dissolution, vapour intrusion risks, and subsurface migration of VOCs like trichloroethylene (TCE) and perchloroethylene (PCE).	Variable soil moisture content, saturated zone thickness and organic matter content can impede the mass transfer of chlorinated solvents, reducing the efficiency of dissolution and vapour intrusion processes.
Mining and tailings sites	Useful for evaluating dissolution of metals and acid mine drainage components into water and gas emissions like sour gas.	Heterogeneous waste composition and gas generation rates can disrupt consistent mass transfer of contaminants, complicating the movement of leachate and gases through the subsurface.
Landfills and waste disposal sites	Mass transfer assesses gas migration (e.g. methane), leachate transport into groundwater, and volatilization of landfill gases.	Seasonal changes in temperature and moisture, and in situ methane generation can alter mass transfer rates of leachate and soil vapour, leading to inconsistent movement of contaminants into groundwater and soil vapour.
Agricultural sites (e.g. fertilizer or pesticide application zones)	Mass transfer quantifies leaching of nitrates, ammonium, and pesticides into groundwater and transport to surface water.	The presence of competing ions or organic residues can inhibit mass transfer of fertilizers and pesticides, slowing their movement into groundwater.
Single-source contaminant plumes	Simple contamination scenarios allow for accurate modelling of advection, diffusion, adsorption, dispersion, and volatilization processes.	Inadequate data on exchange rates, partitioning behaviour, and environmental conditions across multiple media may hinder accurate mass transfer modelling of contaminants.
Sites with minimal media interaction	Simpler systems allow for more reliable mass transfer modelling.	Static site conditions may fail to capture dynamic mass transfer processes, such as volatilization or dissolution over time.
Spills and leaks (e.g. oil spills, produced water spills, pipeline ruptures)	Mass transfer predicts the movement of dissolved hydrocarbons or VOCs into groundwater and air during spills.	Rapid spill evolution and incomplete containment data can limit mass transfer assessment, affecting the tracking of contaminant movement.

Type of Site	Reason	Limitations
Contaminated groundwater plumes	Key to modelling advection, diffusion, adsorption, dispersion, and volatilization of contaminants in groundwater systems.	Aquifer heterogeneity and unknown recharge rates can reduce the reliability of mass transfer predictions, especially for long-term plume stability.

Table 6-4: Unsuitable Sites for Mass Transfer Assessment

Type of Site	Reason
Sites with strongly adsorbed contaminants (e.g. PAHs, PCBs)	Mass transfer is negligible because these contaminants strongly adsorb to soils or sediments and do not move freely.
Sites with low-solubility contaminants (e.g. heavy hydrocarbons, precipitated metals)	Limited relevance since these contaminants have low solubility and volatility, making mass transfer negligible.
Sites with extensive biological or abiotic processes	Highly dynamic or unpredictable processes (e.g. rapid microbial degradation or variable chemical reactions) complicate accurate predictions.
Complex sites with multiple contaminant sources	Overlapping sources (e.g. industrial zones with mixed chemical waste) make it difficult to isolate and model mass transfer processes. However, in some cases, this complexity may lead to conservative outcomes, such as when assessing PCE and its daughter products.
Highly heterogeneous sites with variable media properties	Heterogeneity in soil and complex flow patterns introduces significant uncertainty in mass transfer modelling.
Sites with non-migratory contaminants	Substances like barite microplastics or low solubility synthetic polymers remain stationary and do not interact with surrounding media.
Frozen or permafrost-contaminated sites	Mass transfer processes are negligible in frozen media, where contaminant movement is dominated by freeze-thaw cycles rather than advection or diffusion.

6.6 Relationship to Alberta Policy

6.6.1 Current Status

Mass transfer assessments as a tool in contaminated sites investigation, remediation and risk assessment is currently recognized within current Alberta policy as summarized below.

- Direct measurements of mass transfer between media are required by the ESA guidance (AEPA 2024c) including when mandatory Tier 2 triggers are present at a site (AEPA 2024a; 2024b). Examples of directly measuring mass transfer may include groundwater sampling, soil vapour sampling, porewater sampling, surface water sampling and sediment sampling.
- Current ESA guidance allows for mass flux to be utilized to support CSM development (AEPA 2024c). Mass transfer assessments can be used to inform mass flux calculations.
- While not explicitly documented within Alberta written policy and guidance documents, both geophysical assessments and tracer testing to quantify mass transfer have a precedent of being acceptable lines of evidence to inform CSM development, remedial planning and site-specific risk assessment.
- The standard Tier 1 and Tier 2 models for groundwater transport and vapour intrusion make simplifying assumptions about mass transfer to estimate soil to groundwater, groundwater to

surface water and soil/groundwater to soil vapour / indoor air transport (AEPA 2023; 2024a; 2024b). Alternative models are also permitted within risk assessment with appropriate consultation (AEP 2023).

- Leachability testing of soil and/or sediments is completed for purposes of waste characterization (Alberta Environmental Protection 1996).
- While not explicitly documented within Alberta written policy and guidance documents, mass transfer has precedent of being an acceptable line of evidence to inform site-specific risk assessment, particularly when used to inform mass flux / mass discharge calculations and/or when tissue sampling (e.g. vegetation, fish) is used to inform uptake through the foodchain by higher trophic level receptors.
- While not explicitly documented within Alberta written policy and guidance documents, total mass has precedent of being an acceptable input in ROAs and RAPs including to monitor remedial performance, assess NAPL plume stability, and monitor NSZD and natural attenuation processes. NAPL plume stability and natural attenuation assessments are documented as acceptable lines of evidence to support risk assessment and long-term risk management (AEP 2017; 2023).
- Risk assessments are expected to evaluate both direct and indirect exposure pathways under current conditions and in future (AEP 2023; AEPA 2023). Existing guidance (AEP 2023) references use of cross-media partitioning, which includes an assessment of mass transfer, to quantify current and future exposures considering contaminant fate and transport, and receptor exposure pathways.
- Risk management plans are required to explicitly identify site-specific conditions where contaminant concentrations could affect how contaminants partition in environmental media (AEP 2017). While this does not explicitly specify that mass transfer assessments are required, it is inferred that mass transfer assessments could be used to address this requirement.
- While not explicitly documented within Alberta written policy and guidance documents, mass transfer assessments may be included in complex fate and transport modelling. Complex fate and transport models are documented as an acceptable line of evidence to support risk assessment and long-term risk management (AEP 2023).

6.6.2 Gaps in Alberta Policy and Opportunities for Improvement

Mass transfer assessments of contaminants as a tool in contaminated sites investigation, remediation and risk assessment is currently recognized and required by current Alberta policy and guidance. Gaps in Alberta's written policy and guidance are limited but include:

- guidance on the acceptability of non-standard laboratory tests (e.g. column tests, bioaccumulation tests); and
- the degree of characterization that is required for receiving environments. In many jurisdictions, requirements for spacing of lateral and vertical delineation points, seasonality of sampling and other components of characterization are more prescriptive.

6.7 Costing

Estimating the cost of a mass transfer assessment for a standard oil and gas lease in Alberta (see Section 1.3.1 for definition and assumptions) varies based on several factors, including the specific assessment methods employed, the site's geological and hydrological characteristics, the extent of contamination, and the regulatory requirements. A comprehensive assessment typically involves a combination of field studies, laboratory analyses, and modelling approaches. As such,

mass transfer assessments for a standard oil and gas lease can vary, as outlined below in Table 6-5, below.

Table 6-5: Estimated Cost for a Mass Transfer Assessment for a Standard Oil and Gas Lease

Task	Description	Cost Estimate
Project Planning and Data Review	Review CSM (10–20 wells), plan data collection for mass transfer (e.g. sampling points, lab tests); and coordinate logistics (lab, equipment).	$2,250 - $3,000
Soil Properties and Tortuosity	Collect and analyse 5 soil cores for grain size, porosity, permeability, and tortuosity via lab tests (e.g. sieve analysis, permeameter).	$1,500 - $2,000
Concentration Gradient Data	Collect groundwater samples from 10 wells (5 source, 5 downgradient) for 20 COPCs (PHCs, PAHs, metals, salinity, VOCs).	$750 - $1,000
Mass Transfer Coefficients	Conduct batch experiments on 5 soil-water samples to derive site-specific coefficients for volatilization and soil-water exchange.	$2,500 - $3,500
Boundary Conditions - Hydraulic Data	Measure hydraulic conductivity (5 slug tests) and water levels (10 wells, 1 day) to refine flow boundaries and gradients; includes piezometer rental and crew.	$4,000 - $5,500
Process-Specific Field Data	Perform 3 column studies with site soil/groundwater to quantify advection, dispersion, and sorption/desorption rates.	$4,500 - $5,500
Redox and Biogeochemical Data	Analyse 5 groundwater samples for redox conditions, pH, dissolved oxygen, electron acceptors, and total organic carbon.	$1,000 - $1,500
Field Labor and Equipment	Deploy field crew (2 technicians, 2 days) for sampling, slug tests, and water level measurements; equipment rental (meters, coring tools, vehicles).	$4,000 - $6,000
Data Compilation and Reporting	Compile mass transfer rates (e.g. diffusion, advection) and reporting.	$5,000 - $6,500
Project Management	Oversee field activities (2 days), lab submissions, and reporting; includes scheduling, QA/QC, and client/regulatory communication.	$3,000 - $4,500
Total Estimated Cost		**$28,500 – $39,000**

These estimates are approximate and can vary based on site-specific conditions, regional labor rates, and the complexity of the contamination. Costs will be reduced if data are collected concurrently with CSM development and/or execution of other field programs.

6.8 Summary

Mass transfer assessments evaluate the movement of contaminants across environmental media using methods like Fick's Laws of Diffusion, mass transfer coefficients, empirical models, and experimental techniques. These methods require detailed data, including fluid properties (viscosity, density, solubility), concentration gradients, interface characteristics, and site-specific factors like tortuosity and redox conditions, often collected through laboratory tests and in situ measurements. Costs vary depending on the complexity of the site and chosen approach, with laboratory experiments being less expensive but less representative than field studies, which incur higher costs due to equipment, monitoring wells, and geophysical surveys. In contaminated site management, these assessments predict contaminant fate and transport, informing risk

assessments, remediation designs, and strategies to mitigate risks like groundwater contamination, enhancing long-term human health and environmental protection.

7. Mass Loading to Sensitive Receptors

7.1 Description

Mass loading refers to the total mass of a contaminant entering or migrating through an environmental medium, such as soil, sediment, groundwater, surface water, soil vapour, and air, over a defined period (USEPA 2001a). As such, it provides insight into the total contaminant burden impacting receptors or migrating across property boundaries (USEPA 2001a). Mass loading is similar to mass discharge in that both represent the movement of contaminants across system boundaries and involve the summation of mass flux. However, mass loading typically refers to the rate at which contaminants enter the system, whereas mass discharge refers to the rate at which contaminants exit the system. In a steady-state system, where the amount of contaminant entering the system equals the amount exiting, mass discharge would equal mass loading. However, in dynamic systems, factors like retention, transformation and storage can cause mass loading and mass discharge to differ (ITRC 2010b).

Mass loading is influenced by source characteristics, hydrogeological conditions, and characteristics of the receiving environment. Factors of importance include contaminant concentration, mass and solubility, contaminant release rates, groundwater flow velocity, hydraulic conductivity, hydraulic gradient, organic carbon content, porosity and permeability of the subsurface medium (e.g. soil, sediment, or aquifer), and the cross-sectional area perpendicular to contaminant flow (USEPA 2001a; Looney et al. 2006). Mass loading is determined by transport mechanisms such as advection, diffusion, and dispersion, as well as attenuation processes like biodegradation, sorption, and volatilization, which influence the movement and reduction of contaminants through environmental media over time (CCME 2016).

In contaminated site management, mass loading is used to evaluate source zone strength, predict contaminant plume behaviour, and design remediation strategies. For example, in groundwater systems, mass loading helps assess the effectiveness of pump-and-treat systems or natural attenuation by tracking decreases in contaminant flux over time, indicating the amount of mass extracted or reduced from the original source. Additionally, mass loading assessments are essential when evaluating risks to downgradient receptors, such as drinking water wells or surface water bodies, where contaminant migration could pose ecological or human health impacts. Calculations typically involve measuring contaminant concentrations and groundwater flow rates across a defined cross-sectional area, with adjustments for factors such as matrix porosity and plume heterogeneity.

One key advantage of mass loading over concentration-based assessments is its ability to account for contaminant flux, rather than focusing solely on localized contaminant levels. In concentration-based assessments, a site may be flagged as non-compliant if contaminant concentrations exceed regulatory guidelines, even if the contaminant mass flux is minimal and poses little risk to downstream receptors. Conversely, a site with lower concentrations but high groundwater flow rates could transport a significant contaminant mass to a receiving environment, posing a more substantial risk to receptors despite compliance with concentration guidelines. This distinction is

particularly important in systems with variable groundwater velocities, fluctuating flow conditions, or large contaminant plumes where concentration data alone may not capture the full extent of contaminant migration.

A reduction in mass loading can indicate effective source control or successful implementation of remediation measures, even if contaminant concentrations in localized hotspots remain elevated. However, accurately quantifying mass loading can be challenging due to site heterogeneity, temporal variations in contaminant release rates, and limitations in available site characterization data. Advanced modelling tools and high-resolution site characterization techniques are often employed to refine mass loading estimates and better predict contaminant fate and transport. Overall, mass loading integrates source mass, transport dynamics, and receptor exposure pathways into a single quantitative measure that informs risk management and remediation decision-making.

7.2 Media Considered

Mass loading analyses consider multiple environmental media through which contaminants migrate, as these media serve as pathways for contaminant transport and receptor exposure. The following presents mass loading considerations for each relevant environmental medium, highlighting the pathways through which contaminants migrate and factors influencing their transport, persistence, and exposure risks.

- **Soil:** Soil acts as both a source and a transport medium for contaminants. Contaminants introduced to the soil can migrate vertically or laterally, influenced by factors such as permeability, sorption capacity, and moisture content. Soil characteristics, including grain size distribution, organic carbon content, and porosity, affect contaminant retention and mobility. Mass loading in soil assessments often involves evaluating leaching potential, which determines the likelihood of contaminants reaching groundwater.
- **Groundwater:** Groundwater serves as a primary transport medium for dissolved-phase contaminants. Contaminants migrate through groundwater via advection, dispersion, and diffusion, with mass loading assessments quantifying the contaminant flux moving through aquifers. Parameters such as hydraulic conductivity, hydraulic gradient, and effective porosity influence groundwater contaminant transport. Groundwater mass loading is critical for assessing risks to downgradient receptors, including drinking water wells and surface water bodies.
- **Surface Water:** Surface water can act as both a receptor and a transport medium for contaminants. Contaminants enter surface water through direct discharge, stormwater runoff, groundwater discharge, or atmospheric deposition. Mass loading calculations in surface water environments integrate flow rates and contaminant concentrations to determine overall contaminant mass entering aquatic systems. Factors such as dilution, volatilization, and sedimentation influence contaminant persistence and bioavailability.
- **Sediment:** Sediment functions similarly to soil but is specific to aquatic environments, where it can accumulate contaminants from surface runoff, industrial discharge, or historical deposition. Contaminants in sediment can undergo resuspension due to hydrodynamic forces, leading to secondary contamination of water bodies. Mass loading assessments in sediment involve measuring contaminant concentrations and sediment transport rates to estimate potential exposure risks to aquatic life and human receptors.

- **Soil Vapour:** Soil vapour represents the gas-phase migration of volatile and semi-volatile subsurface contamination sources. Mass loading assessments for soil vapour focus on vapour-phase diffusion and advection, particularly in scenarios where vapour intrusion into buildings poses risks to indoor air quality. Parameters such as soil permeability, temperature, and organic carbon content influence vapour migration rates. Mass loading calculations consider vapour flux from subsurface sources and its potential to accumulate in enclosed spaces, posing exposure risks to human receptors.
- **Air:** Air serves as a medium for the atmospheric transport of contaminants, particularly those released through volatilization, combustion, or industrial emissions. Mass loading assessments for air include evaluating contaminant flux from soil or water surfaces, as well as direct emissions from anthropogenic sources. Atmospheric dispersion models may be used to predict contaminant transport and deposition rates, which inform exposure assessments for human and ecological receptors.

7.3 Approach

Mass loading assessment for a contaminated site is determined by first gathering hydrogeological data, including groundwater flow velocity, hydraulic conductivity, hydraulic gradients, and contaminant concentrations, along with site characteristics such as porosity and permeability. These data are integrated with historical information where available. Mass flux, the rate at which contaminants are transported through the environment (see Section 2.1), is then determined (USEPA 2001a; USEPA 2003). The total mass loading, or the amount of contaminant mass reaching a receptor over time, is then determined by summing the mass flux across the site and accounting for attenuation processes such as biodegradation, sorption, dispersion, dilution, or volatilization, where possible (USEPA 2001a). Thus, integrating mass flux from multiple monitoring wells and applying attenuation factors to contaminant concentrations during transport provides a more accurate estimate of contaminant loading to sensitive receptors, such as groundwater wells or surface water bodies, over the long term.

A numerical model such as Hydrological Simulation Program – FORTRAN HSPF) model (USEPA 2018), MODFLOW (USGS 2022) or MT3DMS (Zheng et al. 2012) may be used to simulate groundwater flow and contaminant transport, integrating mass flux estimates and attenuation effects to provide a detailed picture of contaminant movement and mass loading (USEPA 2003). Calibration of the model with existing data provides more accurate predictions of fate and transport. Uncertainty analysis is an important component of model development, allowing for practitioners to better understand potential variations in contaminant transport and validate model results.

7.4 Data Requirements

Mass loading assessments require additional data beyond those collected for a robust CSM to refine contaminant flux estimates and receptor impact evaluations. The following data may be required:

- Hydraulic Connectivity and Pathway Variability:
  - Detailed assessment of preferential flow paths and their spatial variability influencing contaminant migration and receptor exposure.

- Vadose Zone Transport Properties:
  - Permeability and moisture content data in the unsaturated zone to assess influences on contaminant migration and mass loading to groundwater and soil vapour.
- Cross-Sectional Contaminant Flux Quantification:
  - Hydraulic gradient, aquifer thickness, groundwater velocity, and hydraulic conductivity data to estimate groundwater flow rates across defined transects, and in surface water systems, channel cross-sectional profiles, velocity distributions, and depth-integrated contaminant concentrations to quantify total contaminant flux across different flow regimes.
- Surface Water Flow and Dispersion Patterns:
  - Measurements of flow velocity, dilution factors, and contaminant dispersion patterns in surface waterbodies receiving groundwater or surface runoff contamination.
- Sediment Transport and Resuspension Dynamics:
  - Data on sediment erosion, deposition, and resuspension rates, including bed shear stress, sediment grain size distribution, settling velocity, and turbidity under varying hydrodynamic conditions (e.g. storm events, tidal fluctuations, or seasonal flow changes / freshet) to assess contaminant remobilization and secondary loading.
- Mass Flux at System Interfaces:
  - Measurements of contaminant mass flux (integrating flow rate and concentration) at points where contaminants enter a receiving environment, such as groundwater discharge into surface water, vapour migration into indoor air, or sediment transport into aquatic systems.
- Vapour Intrusion Flux Measurements:
  - Quantification of vapour-phase contaminant migration into indoor air from subsurface sources, including soil gas sampling and building-specific entry parameters (e.g. pressure differentials, building ventilation rates).
- Time-Series Contaminant Concentrations:
  - High-resolution temporal data from monitoring wells, surface water, soil vapour, or air to assess variations in seasonal and transient changes in loading rates.
- Meteorological Data for Airborne Transport:
  - Wind speed, atmospheric stability, and deposition rates to assess airborne contaminant loading to receptors.
- Airborne Contaminant Dispersion:
  - Measurements of atmospheric dispersion parameters and deposition rates to assess mass loading to and from air for VOCs, semi-volatile organics, and contaminants transported as aerosols.
- Soil and Sediment Geochemistry:
  - Data on organic matter content, mineralogy, cation exchange capacity, and sorption/desorption coefficients to evaluate contaminant partitioning between solid and aqueous phases and potential for delayed loading due to desorption.
- Porewater Chemistry:

- Measurements of redox conditions, pH, ionic strength, and geochemical parameters to refine contaminant attenuation estimates influencing mass loading via speciation, solubility, and mobility.

- Surface Water Geochemistry:
  - Measurements of pH, redox conditions, and major ion chemistry in surface water to assess contaminant speciation, interactions with suspended particulates, and potential for transformation or precipitation.
- Attenuation Rate Parameters:
  - Site-specific degradation rates, sorption coefficients, and volatilization rates to refine estimates of contaminant reductions during transport.
- Biodegradation Kinetics:
  - Site-specific microbial activity data (e.g. degradation rate constants, microbial population estimates) to improve mass reduction estimates through natural attenuation processes.

7.5 Applications

Mass loading analysis helps provide insights into the total contaminant burden impacting receptors and receiving environments, or migrating across property boundaries, providing essential data for risk assessment, regulatory compliance, remediation strategies, and long-term site management. Table 7-1 outlines key applications of mass loading, demonstrating how this tool supports effective decision-making in managing contaminated sites. Table 7-2 and Table 7-3 outlines site types where mass loading is either beneficial or not required.

Table 7-1: Applications of Mass Loading in Contaminated Site Management

Application	Description	Key Uses
Risk Assessment	Mass loading helps quantify contaminant transport to assess potential risks to human health and the environment.	• Estimating exposure risks to sensitive receptors (e.g. drinking water sources, residential areas, surface water bodies). • Supporting risk-based site closure decisions.
Groundwater Management	Mass loading helps evaluate contaminant movement through groundwater to confirm drinking water supplies and nearby wells remain protected.	• Identifying areas where contaminant concentrations exceed regulatory limits. • Determining the need for remedial action or monitoring well placement.
Remediation Strategy Design	Mass loading estimates guide the design of remedial systems by identifying areas with more impacts and predicting the effectiveness of remediation technologies.	• Informs remediation by quantifying contaminant fluxes to guide treatment, containment, attenuation, and monitoring. • Determining optimal locations for remediation wells. • Evaluating effectiveness of containment or source removal strategies.
Natural Attenuation Assessment	Mass loading is used to determine how natural processes (e.g. biodegradation, sorption) affect contaminant movement and mass reduction over time.	• Assessing whether natural attenuation is a viable remediation option. • Supporting "no action" decisions when mass loading reductions meet regulatory criteria.

Application	Description	Key Uses
Regulatory Compliance	Mass loading calculations are required for demonstrating compliance with environmental regulations, particularly for long-term monitoring or site closure.	• Verification that contaminant levels remain at or below acceptable concentrations. • Providing evidence for regulatory agencies during site closure or risk mitigation.
Environmental Impact Assessment	Mass loading provides data to assess the broader environmental impact of contamination, including potential effects on ecosystems and surface water bodies.	• Evaluating potential risks to ecosystems such as wetlands, streams, or agricultural land. • Guiding mitigation actions to protect sensitive environmental receptors.
Monitoring and Long-Term Management	Ongoing mass loading analysis supports the tracking of contaminant movement, evaluating trends, and adjusting site management strategies accordingly.	• Planning for future sampling and monitoring activities. • Adjusting remediation efforts based on changing mass flux patterns. • Tracking plume migration over time.

Table 7-2: Relevant Sites for Determining Mass Loading

Type of Site	Reason	Limitations
Sites with single contaminant sources	Easier to quantify mass loading from a single point source, such as a leaking underground storage tank (UST).	May not account for non-point sources or background contamination, leading to over- or underestimation of total mass loading.
Gas plants with airborne particulate or VOC emissions	Potential mass loading of airborne particulates or VOCs to nearby sensitive receptors (e.g. residential areas, schools).	Variable atmospheric conditions can complicate the accurate assessment of mass loading.
Sites with persistent contaminants (e.g. PCBs)	Applicable due to the persistence of contaminants, which allows them to migrate over long distances and creates the potential for plumes to reach groundwater-sensitive receptors, such as drinking water wells.	Subsurface heterogeneity can make it difficult to accurately quantify migration rates and predict long-term transport.
Sites near sensitive ecosystems or receptors	Useful for quantifying containment transport to potential sensitive receptors, including wetlands, aquatic ecosystems, or populations relying on nearby resources.	Natural attenuation and complex ecosystem interactions can alter contaminant fate and transport, making mass loading estimates uncertain.
Multiple-source industrial sites	Relevant for cumulative risk assessment, as mass loading helps identify contributions from each source to sensitive receptors.	Complexity increases with multiple sources, leading to potential overlap or interference in measuring individual contributions accurately.
Sites with contaminated groundwater	Relevant when groundwater contamination threatens downgradient receptors and receiving environments such as private wells or wetlands.	Groundwater flow dynamics, including seasonal fluctuations and preferential pathways, can complicate mass loading calculations.
Sites with active contaminant transport pathways	Relevant when mechanisms like groundwater flow, surface water movement, or air dispersion actively carry pollutants toward sensitive receptors, increasing the risk of exposure.	Transport pathways can be variable and influenced by external factors (e.g. climate conditions, land use changes), affecting mass loading predictability.

Table 7-3: Unsuitable Sites for Determining Mass Loading

Type of Site	Reason
Small, isolated sites with minimal contamination	Limited contamination means mass loading analysis may not be necessary.
Sites without nearby receptors	Not applicable if there is no potential for human or ecological exposure.
Sites with non-mobile contaminants	For contaminants with minimal mobility (e.g. PAHs strongly adsorbed to soil), mass loading to receptors is not a concern.
Non-volatile contaminants far from receptors	Unnecessary when contaminants are non-volatile, immobile, and lack migration pathways to sensitive receptors (e.g. heavy PAHs in stable soil matrices).
Sites remediated or controlled	Unsuitable if remediation has effectively eliminated migration pathways, removing the need for mass loading assessment.
Single-phase liquid releases with no receptors	Unsuitable where contamination remains localized and there are no pathways or receptors of concern (e.g. minor contained spill).

7.6 Relationship to Alberta Policy

Mass loading to sensitive environments generally considers the other mass-based tools described above such as total mass, mass partitioning, mass flux, mass discharge and/or mass transfer. As such, the current status, gaps in Alberta Policy and opportunities for improvement are consistent with those described above.

7.7 Costing

The following table outlines the estimated costs for conducting mass loading for a standard oil and gas lease in Alberta (see Section 1.3.1 for definition and assumptions). The analysis will involve evaluating mass flux and contaminant movement through soil and groundwater, utilizing existing site data and field measurements.

Table 7-4: Estimated Cost for a Mass Loading Analysis at a Standard Oil and Gas Lease

Task	Description	Cost Estimate
Project Planning and Data Review	Review CSM (10–20 wells), plan data collection for mass loading (e.g. receptor pathways, sampling points); coordinate logistics (lab, equipment).	$2,250 - $3,000
Hydraulic Connectivity and Pathway Variability	Conduct 5 slug tests to assess preferential flow paths and variability in hydraulic conductivity.	$3,000 - $4,000
Vadose Zone Transport Properties	Collect and analyse five soil cores from the unsaturated zone for permeability and moisture content via lab tests (e.g. permeameter, moisture analysis).	$1,500 - $2,000
Cross-Sectional Contaminant Flux Quantification	Measure groundwater velocity and hydraulic gradient in 10 wells (piezometers, 1-day effort) and sample for 20 COPCs.	$3,000 - $4,000
Time-Series Contaminant Concentrations	Collect quarterly groundwater samples from five key wells over 1 year (four events) to assess temporal variability.	$2,000 - 2,500
Soil and Sediment Geochemistry	Analyse five soil samples for organic matter content, cation exchange capacity, and sorption/desorption coefficients.	$1,000 - $1,500
Porewater Chemistry (if available)	Extract and analyse porewater from five soil cores for redox conditions, pH, and ionic strength to assess attenuation.	$1,500 - $2,000

Task	Description	Cost Estimate
Attenuation Rate Parameters	Conduct batch experiments on three soil-groundwater samples to estimate site-specific sorption and volatilization rates.	$2,000 - $3,000
Biodegradation Kinetics	Analyse five groundwater samples for microbial activity (e.g. degradation rate constants via molecular probes).	$1,500 - $2,000
Field Labor and Equipment	Deploy field crew (two technicians, two days) for sampling, slug tests, and water level measurements; and equipment rental (meters, coring tools, vehicles).	$5,000 - $6,000
Data Compilation and Reporting	Assess mass loading data and prepare report.	$5,000 - $6,500
Project Management	Oversee field activities (2 days), lab submissions, and reporting; includes scheduling, QA/QC, and client/regulatory communication.	$3,000 - $4,500
Project Planning and Data Review	Review CSM (10–20 wells), plan data collection for mass loading (e.g. receptor pathways, sampling points); coordinate logistics (lab, equipment).	$2,250 - $3,000
Total Estimated Cost		**$30,750 - $41,000**

This cost is for a one-time evaluation; ongoing monitoring for mass loading is optional and would approximately cost an additional $15,000 - $30,000 per year, based on the need for annual sampling, analysis, and reporting to validate contaminant movement and site conditions over time. These estimates are approximate and can vary based on site-specific conditions, regional labor rates, and the complexity of the contamination. Costs may be reduced if data are collected concurrently with CSM development and/or execution of other field programs.

7.8 Summary

Mass loading assessments measure mass flux—the product of contaminant concentrations and flow rates across environmental media like groundwater—to quantify the rate of contaminants entering a system toward sensitive receptors or receiving environments, often aided by models such as MODFLOW to simulate transport and attenuation. Data requirements include detailed hydrogeological parameters (e.g. hydraulic conductivity, groundwater velocity), time-series contaminant concentrations, and site-specific attenuation factors (e.g. biodegradation rates, sorption coefficients), necessitating extensive field sampling and laboratory analysis that can increase costs, particularly when advanced modelling or high-resolution characterization is involved. Mass loading assessments aid contaminated site management by gauging exposure risks to sensitive receptors or receiving environments and evaluating remediation success, thereby guiding strategies to safeguard downgradient receptors.

8. Mass Balance Modelling

8.1 Description

Mass balance is defined as a simple accounting process that tracks the inputs (loading), outputs (releases), accumulation, transformation (conversion, destruction, or creation), and discharge of a substance within a system, such as an aquifer or a segment of a groundwater plume (Chappelle et al. 2004; Looney et al. 2006). By systematically quantifying processes such as sorption, biodegradation, volatilization, and dispersion, mass balance modelling provides a comprehensive understanding of contaminant behaviour and fate. For instance, in groundwater systems, mass balance modelling evaluates whether a contaminant plume is expanding, stabilizing, or contracting, offering insights for design of effective remediation strategies (USEPA 1998b; Chapelle et al. 2004; Looney et al. 2006). This framework can also integrate results from the previously mentioned mass-based approaches, encompassing contaminant quantification, distribution, transport, and transfer, to provide a comprehensive assessment of contaminant dynamics.

The principle of mass balance can be expressed mathematically as the relationship between the rate of mass entering, the rate of mass leaving, the rate of mass accumulation, and the rate of mass destruction or transformation (USEPA 2001a). At steady-state conditions, the mass entering the system equals the mass leaving the system plus mass that is being stored or degraded. For contaminants in groundwater, this balance is often described using the integrated mass flux (iMF) concept, which quantifies the total contaminant mass migrating across a transect over time (Looney et al. 2006).

Two primary approaches are used to evaluate mass balance: empirical and deterministic (Looney et al. 2006). Empirical approaches rely on observed data, such as field measurements of contaminant concentrations and fluxes, to directly quantify inputs and outputs. This approach is particularly effective when sufficient historical data are available, as it reflects real-world conditions and integrates the cumulative effects of attenuation mechanisms (Looney et al. 2006). The deterministic approach, defined as a process in which events follow a consistent and predictable sequence, uses mathematical models based on known physical, chemical, and biological processes governing contaminant fate and transport (Looney et al. 2006). These models incorporate variables such as advection, dispersion, sorption coefficients, biodegradation rates, and source decay profiles. While deterministic models offer predictive capabilities and allow scenario testing (e.g. source removal or enhanced attenuation interventions), their reliability is dependent on the accuracy of input parameters. Combining empirical data with deterministic modelling enhances the reliability of mass balance assessments by calibrating predictions against real-world measurements while allowing exploration of future scenarios (USEPA 1998b; Warren et al. 2007).

Mass balance assessments evaluate the total mass of contaminants across different media, accounting for their transport, transformation, and fate over time. Because this method is dynamic, it provides practitioners with a comprehensive understanding of contamination

behaviour, helping predict long-term impacts and inform effective remediation strategies. For example, mass balance models can answer questions such as whether the natural attenuation capacity of a site is sufficient to stabilize a contaminant plume, what removal rates are necessary to meet cleanup goals, and how long remediation efforts are likely to take (Chapelle et al. 2004; DeSimone et al. 1997). While mass balance is more data-intensive and requires complex modelling compared to concentration-based assessments, this approach provides a more accurate picture of environmental risks than evaluations based solely on deterministic measurements of concentration. In contrast, concentration-based assessments focus on point-in-time contaminant levels, often for purposes of demonstrating regulatory compliance. While use of a concentration-based approach provides a simple and rapid method of screening data, it only offers a snapshot of site conditions at a given moment. This limitation may restrict a practitioner's ability to assess seasonal variability, temporal and spatial changes within a contaminant plume, short-term fluctuations that could indicate transient releases or rapid shifts in site conditions, and overall contaminant dynamics. As such, mass balance assessments offer a more holistic view of contamination, providing valuable insights into long-term trends and the broader environmental context that concentration-based assessments may overlook.

8.2 Media Considered

Mass balance modelling evaluates the fate and transport of contaminants across various environmental media to provide a comprehensive understanding of contaminant dynamics within a system. The following environmental media are typically included in mass balance modelling:

- **Soil:** Soil is a primary medium in mass balance modelling, particularly for sites with surface or near-surface contamination. Soil acts as a reservoir for contaminants, where processes such as sorption, biodegradation, and volatilization occur. Contaminant concentrations in soil, along with properties like soil-water partition coefficients and sorption characteristics, are used to quantify how much contaminant mass is retained, transformed, or released into other media like groundwater or air.
- **Groundwater:** Groundwater is a central focus in many mass balance models, especially for aquifer systems or sites with subsurface contamination. Models assess contaminant fate and transport through processes like advection, dispersion, and biodegradation, using data such as groundwater flow rates, hydraulic conductivity, permeability, and porosity. The integrated mass flux (iMF) concept often quantifies contaminant movement across groundwater transects, helping to determine whether a plume is expanding, stabilizing, or contracting.
- **Surface Water:** Surface water is considered in mass balance modelling when contaminants migrate from groundwater or soil into wetlands, rivers, lakes or streams. This medium is critical for understanding downstream impacts and potential exposure risks to aquatic ecosystems or human receptors. Data on surface water include contaminant concentrations, flow rates, and interactions with sediments, as well as processes like dilution and volatilization at the air-water interface.
- **Sediments:** Sediments in surface water bodies or depositional zones are included as a medium because they can act as both a sink and a source of contaminants. Persistent contaminants, such as PCBs, often accumulate in sediments, where they may undergo slow degradation, suspension and redistribution or remobilization. Sediment-water partition coefficients and sediment contaminant concentrations are key parameters in modelling these interactions.

- **Soil Vapour:** Soil vapour facilitates the migration of volatile contaminants, such as VOCs, from soil or groundwater into the air. Mass balance models account for volatilization processes using data like soil vapour concentrations and air-water mass transfer coefficients. This medium is particularly relevant for assessing risks of vapour intrusion into buildings or atmospheric releases.
- **Air:** The atmosphere is considered in mass balance modelling for airborne contaminants, including particulate-bound forms and volatile emissions, especially in studies near point sources or when volatilization or particle transport from soil, groundwater, or surface water is significant. Atmospheric dispersion, deposition rates, and air-water exchange processes are quantified using meteorological data such as rainfall, temperature, and volatilization mass transfer coefficients. This medium is used to evaluate exposure risks through inhalation or deposition onto other surfaces.

8.3 Approach

Conducting a mass balance model for a contaminated site requires a systematic approach that is based on the principal of conservation of mass. This method involves evaluating the inputs, outputs, and changes in contaminant mass over time (USEPA 1998b; Looney et. Al 2006). Mass balance models can be tailored for contaminants, where inputs include contaminant sources and their transformation products, outputs include removal mechanisms, and changes in storage reflect accumulation or degradation within the site. Mass balance modelling is crucial for assessing the extent of contamination, determining remediation strategies, and predicting future conditions. The following section outlines the method for developing a mass balance model for a contaminated site.

The process of mass balance modelling begins with contaminant identification and source characterization, including defining contaminants (e.g. PHCs, heavy metals, VOCs) and their sources, such as sumps, flare pits, spills, leaks, or historical land use. The spatial and temporal boundaries of the system are then defined. Spatial boundaries outline the physical extent of elevated contaminant concentrations, including the vertical and lateral extent of impacted soils/bedrock, groundwater plumes and areas where receptors could be exposed to or affected by the contaminants. Temporal boundaries are set to ensure the assessment captures the full lifecycle of contamination, incorporating historical and projected future conditions (Fujinaga et al. 2012).

Data collection is tailored to the complexity of the site, the nature and extent of contamination, and the temporal dynamics influencing contaminant behaviour. A variety of datasets are required to inform the mass balance model, including those that are readily available as part of typical site characterization activities, and those that are collected to support the model as follows:

- **Environmental Monitoring Data:** Contaminant concentrations in soil, groundwater, surface water, sediments, and soil vapour; spatial and temporal distribution of contaminants and associated degradation products; and background levels of contaminants and electron acceptors.
- **Hydrological and Geological Data:** Groundwater flow rates and velocities; aquifer dimensions (e.g. depth, length, width, thickness); hydraulic conductivity; permeability; porosity; water table gradients and flow direction(s).

- **Chemical Properties:** Partition coefficients (e.g. soil or sediment-water, air-water, organic carbon); biodegradation and reaction rate constants; solubility and volatility; diffusion coefficients.
- **Sorption and Retardation Characteristics:** Sorption coefficients and retardation factors for contaminants and interacting ions.
- **Source Information:** Mass loading rates, concentration of contaminants at the lateral and vertical extent of the source, and source characteristics (e.g. point or non-point, continuous or episodic release).
- **Meteorological Data:** Rainfall, temperature, and atmospheric deposition rates; volatilization mass transfer coefficients for air-water exchanges (USEPA 1998b; Chapelle et al. 2004; Looney et al. 2006).

The specific mass balance equation for the system is then established based on the defined inputs, outputs, and transformations. This can generally be stated as follows:

$$\textit{Contaminant Input} - \textit{Contaminant Output} + \textit{Generation} - \textit{Consumption} = \textit{Change in Contaminant Storage}$$

where:

Contaminant Input = The sum of contaminant loading from various sources (direct discharges, runoff, etc.).

Contaminant Output = The amounts leaving the system through processes such as natural attenuation, remediation techniques, or transport to other media.

Generation = New contaminants formed through chemical reactions or processes occurring in situ, such as biogeochemical transformations.

Consumption = Degradation rates due to biological, chemical, or physical processes that reduce contaminant concentrations. (USEPA 1998b; Looney et. Al 2006)

Each term in the equation corresponds to specific processes, such as inflow from an upstream source, outflow via groundwater discharge, degradation by microbial activity, or accumulation in low-flow zones. The equations are tailored to site-specific characteristics and the data collected during site assessment (USEPA 2001a). Figure 8-1 below provides a visual example of a mass balance for a contaminated site.

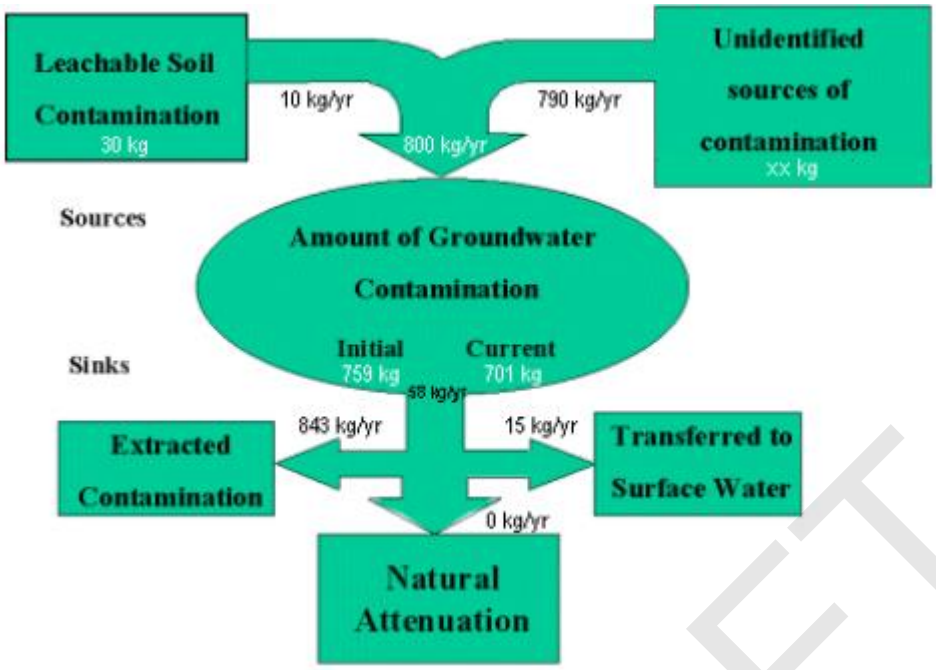

Figure 8-1: Mass balance for a contaminated site using contaminant sources (inputs) and sinks (outputs). Republished from: USEPA 2001a.

Once the equations are established, the next phase is model development using specialized software tools such as MODFLOW (USGS 2022), MT3DMS (Zheng et al. 2012) or other numerical modelling platforms. Site data and formulated equations are entered into the software, and the model is calibrated using observed field data to improve accuracy. Validation follows calibration, where model predictions are compared against independent datasets to verify that the model effectively represents real-world conditions (Looney et al. 2006; Fathi et al. 2021). A sensitivity analysis is also performed to identify parameters that have the greater impacts on model predictions, helping to prioritize data collection efforts and refine assumptions (Wang et al. 2020).

Once the model is calibrated and validated, simulations are performed to forecast contaminant behaviour across different scenarios. These simulations may assess the effectiveness of natural attenuation, predict contaminant migration patterns over time, and/or evaluate the performance of proposed remediation strategies such as pump-and-treat systems or permeable reactive barriers (Looney et al. 2006; Wang et al. 2020; Fathi et al. 2021). The ability to test different scenarios allows decision-makers to weigh the effectiveness, benefits and limitations of each remediation option before implementing interventions.

Outputs of mass balance simulations typically include concentration contour maps, contaminant plume migration trajectories, and hotspot identification for potential exposure risks (USEPA 1998; Looney et al. 2006; Ziegler et al. 2017). These findings are translated into actionable insights for site managers, environmental consultants, and regulators, informing decisions about ongoing monitoring, risk assessment, and cleanup measures.

Mass balance models are continually refined and enhances as the CSM evolves and is updated. This iterative approach improves model accuracy over time and allows for changing site conditions to be adequately addressed (Looney et al. 2006; Warren et al. 2007). As monitoring programs continue, additional field data can be incorporated into the model to recalibrate predictions and improve long-term site management.

Appendix C presents a case study on the application of an empirical mass balance model to quantify contaminant sources in the Lower Passaic River, a designated Operable Unit of the Diamond Alkali Superfund Site in northeastern New Jersey.

8.4 Data Requirements

Mass balance modelling requires additional data beyond those collected for a robust CSM to accurately quantify the movement, transformation, and fate of contaminants in the environment. The following data may be required, informed where applicable by prior mass-based assessments discussed earlier in this report:

- Contaminant Mass Flux and Transformation Data:
  - Mass flux measurements: Quantification of contaminant mass migrating across defined transects to evaluate mass balance at different spatial scales.
  - Degradation and transformation rates: Site-specific biodegradation and abiotic transformation rate constants, including first-order decay rates and half-lives.
  - Reaction stoichiometry: Identification of electron acceptors and degradation byproducts to characterize transformation pathways and confirm attenuation mechanisms.
- Detailed Hydrogeological and Geochemical Data:
  - Groundwater velocity distribution: High-resolution measurements of hydraulic gradients and seepage velocities to improve transport modelling.
  - Fate and Transport Parameters:
    - Hydraulic conductivity and porosity: Site-specific values of hydraulic conductivity and effective porosity to quantify groundwater flow and contaminant mass storage.
    - Dispersivity and diffusion coefficients: Site-specific values for longitudinal, transverse, and vertical dispersivity, along with molecular diffusion coefficients, to refine contaminant plume spreading and dispersion estimates.
    - Retardation coefficients: Site-specific values to quantify sorption and its impact on contaminant transport rates, derived from partition coefficients and organic carbon content.
  - Geochemical conditions: Redox conditions, pH, dissolved oxygen, and major ion concentrations to support evaluations of contaminant degradation and attenuation potential.
    - Natural organic matter content: Characterization of organic carbon in soils and sediments to refine sorption coefficients.
- Source Mass Loading and Release Dynamics:

- Mass loading rates: Quantification of contaminant input from primary and secondary sources, including time-variable releases from non-point sources.
- Source depletion rates: Empirical data on contaminant mass depletion over time to support source decay modelling.
- Vadose zone contributions: Measurements of contaminant flux from the vadose zone to groundwater, including soil-water partitioning coefficients and infiltration rates.

- Air-Water and Soil-Water Partitioning Parameters:
  - Volatilization fluxes: Direct measurement or estimation of volatilization rates from applicable media.
  - Henry's Law constants: Site-specific values for volatile contaminants to improve air-water exchange modelling.
  - Soil-water and sediment-water partitioning: Site-specific partition coefficients to refine mass transfer estimates between media.
- Meteorological and Environmental Forcing Data:
  - Precipitation and recharge rates: High-resolution temporal data on rainfall and infiltration to evaluate recharge impacts on groundwater flow and contaminant transport.
  - Evapotranspiration rates: Estimates of water loss from the subsurface to improve groundwater balance calculations.
  - Temperature variations: Seasonal and diurnal temperature trends affecting contaminant degradation rates and air-water exchange dynamics.

8.5 Applications

Mass balance modelling is used to quantify the movement and distribution of contaminants across various environmental media, aiding in the evaluation and management of contaminated sites. Table 8-1 outlines key applications of mass balance models, their descriptions, and the specific uses that guide effective site management and remediation. Table 8-2 and Table 8-3 outlines site types where mass loading is either beneficial or not required.

Table 8-1: Applications of Mass Balance Models in Contaminated Site Management

Application	Description	Key Uses
Contamination in Environmental Media	Assesses the concentration, distribution, and movement of contaminants in groundwater, soil, and sediments.	• Predict contaminant migration pathways in different media. • Inform ecological risk assessments for aquatic and terrestrial habitats. • Design remediation strategies tailored to each medium. • Estimate mass removal requirements and effectiveness of treatment. • Evaluate long-term environmental impacts and transport dynamics.

Application	Description	Key Uses
Remediation Effectiveness	Analyses the impact of remediation efforts by tracking the reduction in contaminant mass over time.	• Evaluate cleanup success. • Adjust remediation strategies as needed. • Compliance with regulatory standards.
Risk Assessment	Assesses potential risks to human health and the environment by evaluating contaminant mass to determine total exposure levels.	• Estimate exposure risks to human populations. • Set site cleanup goals. • Support regulatory compliance and safety evaluations.
Airborne Contaminants	Tracks the release and movement of airborne contaminants, such as VOCs.	• Predict plume dispersion and concentration. • Assess inhalation risks for nearby populations. • Design air quality monitoring programs.
Wastewater Treatment	Uses mass balance to evaluate the removal of contaminants from wastewater during treatment processes.	• Optimize treatment plant performance. • Evaluate effluent quality. • Maintain compliance with discharge limits.
Source Identification	Identifies the origin and magnitude of contamination by measuring mass inputs and outputs.	• Pinpoint contamination sources. • Prioritize areas for remediation. • Evaluate historical contamination trends.
Long-Term Environmental Monitoring	Monitors changes in contaminant mass over time to track trends and assess long-term environmental impacts.	• Guide long-term site management decisions. • Assess sustainability of remediation efforts. • Evaluate natural attenuation processes.
Landfill Contamination and Leachate Management	Tracks contaminants in landfill leachate and their movement into surrounding environments.	• Assess potential for leachate migration to groundwater. • Design and implement leachate treatment systems or containment barriers. • Evaluate long-term environmental impacts of landfill sites.
Bioremediation and Natural Attenuation	Assesses the mass of contaminants reduced or transformed through biological processes in the environment.	• Estimate the rate of natural attenuation in contaminated media. • Evaluate the effectiveness of bioremediation or natural attenuation strategies. • Support long-term monitoring and optimization of bioremediation projects.

Table 8-2: Relevant Sites for Mass Balance Modelling

Type of Site	Reason	Limitations
Relevant Sites		
Sites with single contaminant sources	Simplifies modelling as there is only one point of origin, enabling precise mass balance calculations.	Assumes no secondary sources or transformations, which may oversimplify real-world complexity and lead to inaccurate mass estimates if additional inputs are present.

Type of Site	Reason	Limitations
Relevant Sites		
Sites with persistent contaminants (e.g. PCBs)	Persistent chemicals remain in the environment for long periods, making mass balance tracking feasible.	Long-term persistence can complicate tracking due to degradation products or changes in chemical behaviour over time, potentially skewing mass balance calculations.
Sites with clear and defined boundaries	Accurate mass balance models require well-defined physical site limits.	Assumptions about uniform conditions (e.g. homogeneous soil or consistent flow) may oversimplify the site, leading to errors in mass balance calculations.
Groundwater contaminated sites with adequate hydrogeological data	Necessary for understanding contaminant transport and flux in aquifers to quantify mass balance.	Seasonal variations or unexpected aquifer heterogeneity can skew mass balance predictions.
Industrial sites with consistent chemical releases	Allows for predictable and measurable contaminant inputs for modelling.	Consistent releases may still have unmonitored variability (e.g. during maintenance or spills), affecting input accuracy.
Sites with extensive historical monitoring data	Historical data supports calibration and validation of mass balance models.	Extensive data may still have gaps or inconsistencies (e.g. changes in sampling methods), complicating model calibration.
Airborne contaminant studies near point sources	Mass balance methods work well for determining emissions and atmospheric dispersion.	Point source proximity may lead to overlooking regional background contributions, skewing emission estimates.
Remediation sites with specific treatment technologies that can be quantified (e.g. pump and treat, SVE)	Enables monitoring of contaminant mass removal over time.	Quantified technologies may face challenges in capturing contaminant mass due to incomplete extraction from low-permeability zones, affecting the accuracy of mass removal assessments.

Table 8-3: Unsuitable Sites for Mass Balance Modelling

Type of Site	Reason
Small-scale sites	Limited data availability, heterogeneity of contamination, and low feasibility of balancing inputs and outputs.
Sites with unknown sources	Mass balance requires well-defined inputs/outputs, which are difficult for sites with unidentified contaminant origins.
Urban brownfields	Mixed-use sites with multiple contaminants and sources make modelling overly complex and unreliable.
Sites with highly reactive contaminants or those with high natural attenuation and biological degradation rates	Short contaminant lifespans and high degradation rates complicate calculations and mass tracking.
Sites with incomplete or poor-quality data	Mass balance modelling relies on precise input/output measurements.
Non-point source pollution	Diffuse contamination from multiple sources, such as general urban runoff, makes it unsuitable for precise mass balancing.

Type of Site	Reason
Highly heterogeneous sites	Data variability in contamination levels, geology, and pathways leads to poor mass balance applicability.

8.6 Mass Balance Modelling

8.6.1 Current Status

The use of mass balance modelling assessments as a decision-making tool in contaminated sites investigation, remediation and risk assessment is currently recognized within current Alberta policy as summarized below.

- The Tier 1 and Tier 2 guidelines require that a mass balance assessment be completed when there is groundwater discharge to a stagnant water body (AEPA 2024a; 2024b).
- The subsoil salinity tool (SST) is a mass balance-based fate and transport guideline calculator (Equilibrium Environmental Inc. 2020).
- While not explicitly documented within Alberta written policy and guidance documents, mass balance has precedent of being an acceptable input in ROAs and RAPs including to monitor remedial performance, assess NAPL plume stability, and monitor NSZD and natural attenuation processes. NAPL plume stability and natural attenuation assessments are documented as acceptable lines of evidence to support risk assessment and long-term risk management (AEP 2017; 2023).
- While not explicitly documented within Alberta written policy and guidance documents, mass balance modelling has precedent of being an acceptable line of evidence to inform site-specific risk assessment, particularly when used to assess potential future risks or inform mass flux / mass discharge calculations.
- While not explicitly documented within Alberta written policy and guidance documents, mass balance may be included in complex fate and transport modelling. Complex fate and transport models are documented as an acceptable line of evidence to support risk assessment and long-term risk management (AEP 2023).

8.6.2 Gaps in Alberta Policy and Opportunities for Improvement

Although mass balance assessment of contaminants is recognized as a tool in contaminated sites investigation, remediation and risk assessment within current Alberta policy and guidance, there are gaps in Alberta's written policy and guidance including what published models are considered acceptable and when published half lives can be reasonably applied to site-specific risk assessments. To address these gaps, it would be beneficial to provide formal written policy and/or guidance that describes:

- What published models are acceptable to AEPA and AER, and the degree of model calibration and field verification that is required to use them;
- When literature derived half-lives can be used to quantify mass balance and field verified rather than the reverse. Note that derivation of site-specific rate constants and estimates of field measured half-lives is highly inaccurate for many sites since in first order decay processes, the rate of decay is higher and slows as source materials are depleted. This is particularly relevant for historical releases where residual concentrations in the environment may be low.

8.7 Costing

The following table outlines the estimated costs for conducting mass balance modelling for a standard oil and gas lease in Alberta (see Section 1.3.1 for definition and assumptions). This estimate assumes mass balance modelling is used to quantify and track the distribution and fate of contaminants across the site, integrating data from various sources, such as groundwater concentrations, soil properties, and contaminant flux. This modelling approach will assess the contaminant mass entering, leaving, and accumulating within the site boundaries.

Table 8-4: Estimated Cost for a Mass Balance Model at a Standard Oil and Gas Lease

Task	Description	Cost Estimate
Project Planning and Data Review	Review CSM (10–20 wells), plan data collection for mass balance (e.g. flux, transformation rates); coordinate logistics (lab, equipment).	$2,250 - $3,000
Contaminant Mass Flux	Measure groundwater velocity and concentrations in 10 wells (piezometers, 1-day effort) for 20 COPCs to quantify flux across transects.	$3,500 - $4,500
Degradation and Transformation Rates	Conduct batch experiments on five soil-groundwater samples to estimate site-specific biodegradation rates and half-lives.	$4,000 - $5,000
Reaction Stoichiometry	Analyse five groundwater samples for electron acceptors (e.g. nitrate, sulphate) and degradation byproducts to confirm transformation pathways; $200–$300/sample, specialized lab tests.	$1,000 - $1,500
Groundwater Velocity Distribution	Perform five slug tests to refine hydraulic gradients and seepage velocities across the site.	$3,000 - $4,000
Transport and Fate Parameters	Collect five soil cores for lab analysis of dispersivity, diffusion coefficients, and retardation coefficients (e.g. permeameter, sorption tests).	$2,000 - $2,500
Geochemical Conditions	Analyse five groundwater samples for redox, pH, dissolved oxygen, and major ions to assess degradation potential.	$1,000 - $1,500
Natural Organic Matter Content	Analyse five soil samples for organic carbon content to refine sorption coefficients.	$750 - $1,000
Source Mass Loading Rates	Sample five wells near source zones quarterly (four events) for 20 COPCs to quantify time-variable inputs.	$2500 -$3000
Source Depletion Rates	Conduct elution tests on 3 source zone soil samples to quantify contaminant depletion rates over time (e.g. leaching experiments).	$1000 - $1,500
Dynamic Sorption/Desorption Kinetics	Perform 3 column studies with site soil and groundwater to measure sorption/desorption rates between phases.	$1,500 - $2,500
Field Labor and Equipment	Deploy field crew (two technicians, four days) for sampling, slug tests, and water level measurements; and equipment rental (meters, coring tools, vehicles).	$8,000 - $12,000
Model Development and Calibration	Develop and calibrate a mass balance model using MODFLOW/MT3DMS, including software licensing, calibration, and validation with field data; includes software costs and professional time.	$30,000 - $60,000

Task	Description	Cost Estimate
Data Compilation and Reporting	Assess mass balance data and prepare report.	$8,000 - $10,000
Project Management	Oversee field activities (3 days), lab submissions, and reporting; includes scheduling, QA/QC, and client/regulatory communication.	$4,000 - $5,000
Total Estimated Cost		**$72,500–$117,000**

These estimates are approximate and can vary based on site-specific conditions, regional labor rates, and the complexity of the contamination. Costs will be reduced if data are collected concurrently with CSM development and/or execution of other field programs.

8.8 Summary

Mass balance modeling employs empirical and deterministic methods to track contaminant inputs, outputs, accumulation, and transformation within environmental systems using tools such as MODFLOW and MT3DMS to quantify processes like advection, dispersion, sorption, and biodegradation. It requires extensive data beyond a typical CSM, including contaminant mass flux, transformation rates, hydrogeological parameters (e.g. hydraulic conductivity, dispersivity), partitioning coefficients, and meteorological data, which increases costs due to the need for detailed field measurements, laboratory analysis, and specialized software expertise. Despite higher costs, these methods enhance contaminated site management by predicting plume behaviour, assessing natural attenuation capacity, evaluating remediation strategies (e.g. pump-and-treat), and providing actionable insights like concentration maps and migration trajectories to inform long-term risk management and cleanup decisions.

9. Contributions In Other Approaches

Mass-based approaches can support other assessment methods, such as the weight of evidence, by providing quantitative data on contaminant distribution and movement, which strengthens the overall risk evaluation process. These approaches help integrate multiple lines of evidence and offer a more comprehensive understanding of contaminant dynamics. The following subsections outline additional assessment methods where mass-based approaches can be applied.

9.1 Weight Of Evidence

The weight of evidence approach is a systematic procedure used to aggregate multiple types of evidence, with the objective of developing a unified conclusion regarding the probability and magnitude of harm (CCME 2020). The approach involves integrating measurement endpoints that are closely linked to lines of evidence for a particular assessment endpoint to evaluate the likelihood and magnitude of ecological risk. First, a preliminary assessment of the relative merit (i.e. providing meaningful information for the evaluation of the assessment point) for each line of evidence is completed using specified decisions, such as Table 1 of the Guidance for Weight of Evidence Approach in Conducting Detailed Ecological Risk Assessments in British Columbia (Scientific Advisory Board for Contaminated Sites in British Columbia [SABCS] 2010). Second, an approach for determining the magnitude of response for each line of evidence is determined. The relative merit and magnitude of response for each LOE is then integrated to draw an overall conclusion as to the potential effects of the contamination being assessed. In general, the first component of a weight of evidence approach is completed *a priori* to limit bias of the assessor, while the second component of a weight of evidence is completed following data collection.

Mass-based approaches can serve as critical lines of evidence in weight of evidence approaches for risk assessments. These approaches provide quantitative and spatial information about contaminant distribution, transport mechanisms, and potential exposure pathways, which complement biological and ecological endpoints in a weight of evidence framework. For example, mass flux data can quantify the rate at which a contaminant plume is migrating through groundwater, while mass discharge can estimate the total contaminant load entering a downstream receptor such as a wetland or stream. When combined with other lines of evidence such as toxicity testing and surface water chemistry, these metrics allow assessors to evaluate whether contaminant concentrations pose an ecological risk and how attenuation processes might reduce exposure over time. In a case where a contaminant plume is migrating towards an aquatic habitat, mass flux and mass discharge measurements could demonstrate whether the contaminant load is sufficient to exceed toxicity thresholds identified in water quality guidelines. By integrating mass based lines of evidence with other environmental data, the weight of evidence approach provides a comprehensive understanding of both the magnitude and likelihood of harm, supporting more informed and defensible risk management decisions.

Appendix B presents a case study using a mass flux-based approach and a weight of evidence framework to assess the short-term and localized aquatic impacts of molybdenum-containing water released in southeast Alberta.

Weight of evidence approaches are permitted within Alberta's regulatory framework (AEPA 2023). However, Alberta's existing guidance and policy is overly conservative which precludes the practical application of this methodology to risk assessment in many scenarios. In addition to the gaps and opportunities for improvement outlined above, policies that require adjustment to make a weight of evidence assessment a useful tool in contaminated sites risk assessment include:

- Flexibility in the definition of biologically active / rooting zone, particularly with site-specific measurements. Currently the biologically active / rooting zone is defined as 1.5 metres for hydrocarbons and salinity and 3.0 metres for other contaminants.
- Broader acceptance of toxicity testing. Current policy communicated by AEPA and AER suggests that toxicity testing can only be used for hydrocarbons, which limits the practicality of using weight of evidence assessment in risk assessment.

9.2 Triad Approaches

The TRIAD method is a comprehensive, site-specific ecological risk assessment framework that integrates multiple lines of evidence to evaluate the risks posed by contaminated sites. Originally developed to enhance decision-making in soil quality management, it combines three distinct but complementary approaches—chemistry, toxicology, and ecology—to provide a robust assessment of contamination impacts (International Organization for Standardization [ISO] 2017). The TRIAD method relies on mass-based assessments, which quantify contaminant behaviour and effects in terms of total mass, distribution, movement, and ecological consequences, enabling a holistic understanding of risk at contaminated sites.

In the chemistry line of evidence, mass-based assessments are used to measure the total mass of contaminants present in environmental media and to determine their bioavailable fractions. The total mass of contaminants provides a baseline for understanding the extent of contamination, while mass partitioning analysis elucidates how contaminants are distributed between phases (e.g. dissolved, sorbed, or volatilized), influencing their availability to biota (Grassi et al. 2022). Additionally, mass balance modeling is employed to predict contaminant fate and transport through environmental compartments, such as soil-to-groundwater pathways or bioaccumulation in food webs (USEPA 1998c). These models incorporate mass loading estimates to assess how contaminant masses might accumulate in sensitive receptors, such as aquatic organisms or terrestrial wildlife, providing a quantitative foundation for risk calculations.

The toxicology component of the TRIAD method utilizes bioassays to measure the actual toxicity of environmental samples collected from the contaminated site. Mass-based assessments enhance this line of evidence by linking observed toxic effects to the mass of contaminants present. Mass flux and mass discharge quantification, for example, estimate the rate at which contaminants are released from a source zone and transported to receptors, offering insights into exposure potential (RIVM 2007). Bioassays, conducted with species across diverse genera, reflect the integrated effects of contaminant mixtures, where mass transfer assessment helps explain how contaminants move from the environment into test organisms (USEPA 1997). By correlating toxicity endpoints (e.g. mortality, growth inhibition) with contaminant mass and bioavailability, this approach ensures that risk estimates are grounded in site-specific conditions rather than theoretical assumptions alone (Grassi et al. 2022).

The ecology line of evidence involves field observations to assess ecological impacts at the contaminated site compared to a reference site. Mass-based assessments are critical here for attributing observed ecological deviations—such as reduced species diversity or altered community structure—to contamination. Mass loading to sensitive receptors quantifies the amount of contaminants reaching key ecological components (e.g. plants, wildlife, wetlands) and helps establish plausible causal links between contaminant mass and ecological effects (ISO 2017). For example, mass discharge from a contaminated soil layer into a nearby stream can be calculated to assess its contribution to observed declines in aquatic biodiversity (USEPA 1998c). By integrating these mass-based metrics with field data, the TRIAD method ensures that ecological risks are evaluated in the context of real-world exposure scenarios, enhancing the reliability of the assessment (RIVM 2007).

The strength of the TRIAD method lies in its integration of these three lines of evidence, with mass-based assessments serving as a unifying thread. Total mass and partitioning analyses from the chemistry component inform exposure estimates, which are validated through toxicology bioassays and correlated with ecological observations. Mass flux, discharge, and transfer assessments bridge the gap between contaminant presence and biological impact, while mass balance modeling provides a predictive tool to evaluate long-term risks and remediation outcomes (Grassi et al. 2022). This iterative process allows for a weight of evidence approach, where discrepancies between lines of evidence can be resolved by refining mass-based inputs or adjusting assessment endpoints (USEPA 1997). Ultimately, the use of mass-based techniques in the TRIAD method ensures a scientifically defensible, quantitative framework for managing contaminated sites and protecting ecological receptors.

The TRIAD method is a well-established weight of evidence approach. Weight of evidence approaches are permitted within Alberta's regulatory framework (AEPA 2023). However as described above, Alberta's existing guidance and policy around toxicity testing is overly conservative which precludes the practical application of this methodology to risk assessment in many scenarios.

9.3 Stochastic and Probabilistic Data Analysis

Probabilistic and stochastic data analysis are both vital in environmental risk assessments. Probabilistic and stochastic-based approaches can significantly enhance these methods by providing more accurate and detailed data on contaminant movement and behaviour. Probabilistic analysis focuses on assessing uncertainty by modelling the likelihood of specific outcomes or events (USEPA 2024a). It uses probability distributions to represent the uncertainty around input parameters, such as contaminant concentrations, mass flux, or environmental conditions. Mass-based approaches, such as mass flux and mass loading, can be integrated into probabilistic models to represent the movement and transport of contaminants through different media. For instance, in a probabilistic risk assessment of groundwater contamination, mass flux (the rate at which contaminants move through a cross-sectional area) and mass loading (the total contaminant mass reaching a receptor) can be assigned probability distributions based on site-specific data or expert judgment. These mass-based metrics help to quantify the potential

contaminant load and its associated risk, and the probabilistic model can simulate a range of possible outcomes, such as the likelihood that the contaminant mass exceeds a certain threshold at a receptor point. This integration helps assess the probability of contamination risks while considering the inherent uncertainty in mass transport parameters. It is recognized at the time of document preparation that Alberta's regulatory framework generally precludes the use of probabilistic risk assessment (AEPA 2023; AEPA 2024b); however, probabilistic methods are applied in select cases and therefore are described herein (e.g. species sensitivity distributions, numerical modelling).

The Australian Government Department of Health (2012) defines stochastic as a random probabilistic phenomenon. As such, stochastic models can have a probabilistic element, such as a Monte Carlo simulation, which characterizes the uncertainty and variability in estimates by sampling the probability distributions for one or more variables within the model (USEPA 2001b). Stochastic models rely on random variables and are ideal for capturing the dynamic and fluctuating nature of environmental systems, including the transport and fate of contaminants. For example, a stochastic simulation of groundwater contamination could incorporate mass discharge data to model how contaminants flow through an aquifer over time, considering random variations in hydraulic conductivity, soil properties, and flow rates. Mass transfer data would also be used to model how contaminants move between soil, water, and air phases, further enhancing the realism of the stochastic model. This allows for the consideration of random processes and system dynamics, providing insights into the long-term behaviour and fate of contaminants in an evolving system. Additionally, basic statistics, such as mean, variance, and standard deviation of contaminant concentrations or mass measurements, are also considered a stochastic approach, as they quantify variability and randomness in environmental data, offering a foundational layer for understanding system behaviour over time.

Both approaches benefit from the use of mass-based approaches. In a probabilistic framework, mass flux, mass partitioning, and total mass of contaminants provide the necessary data to model the movement and distribution of contaminants under uncertainty. In a stochastic model, mass discharge, mass transfer, and mass loading offer input data for simulating the dynamic evolution of contaminant transport, accounting for random fluctuations in system conditions. By incorporating mass-based approaches into both types of analysis, practitioners can gain a more comprehensive understanding of contaminant dynamics and improve their predictions of contamination risk, considering both the inherent uncertainties and the time-dependent behaviour of contaminants.

Probabilistic risk assessment has not been historically permitted by Alberta policy and probabilistic methods such as species sensitivity distributions are generally not accepted unless related to published guidelines or screening levels. Development of species sensitivity distributions based on site-specific species or more relevant and recent toxicity data compared to generic published guidelines are generally not permitted. Stochastic methods are permitted in risk assessment for mobile receptors and development of background levels but are not accepted for immobile receptors. Guidance that improves alignment of AEPA and AER policy with other regulatory jurisdictions would be helpful for operators and practitioners in contaminated sites risk assessment.

10. Comparative Analysis

This section summarizes the mass-based approaches presented in this report, focusing on their roles in evaluating contamination dynamics, guiding remediation, and informing risk assessments to support comparison. The summary provides an overview of the suitability of each approach for contaminated site management, including data needs and a comparative cost analysis.

10.1 Applicability to Contaminated Sites

The table below summarizes how the mass-based methods discussed in this document aid in understanding and managing of contamination. These approaches address key questions regarding contaminant distribution, transport, and associated risks. By connecting each method to the key questions it addresses, along with its practical applications, advantages, and limitations, the table highlights their significance in informing remediation design, risk assessment, and regulatory compliance at contaminated sites.

Table 10-1: Key Questions, Applications, Advantages, and Limitations of Mass-Based Approaches in Contaminated Site Management

Method	Key Questions Answered	Key Applications	Advantages	Limitations
Total Mass of Contaminants	• What is the total amount of contamination present at the site? • How is the contaminant mass distributed across different environmental media? • How much contaminant mass is mobile or bioavailable? • How effective would remediation efforts be?	• Quantify contamination extent and severity. • Inform remediation design and technology selection. • Evaluate risks to human health and the environment. • Monitor remediation effectiveness over time. • Support regulatory compliance and cost estimation.	• Provides a baseline measurement of the extent of contamination. • Useful for setting cleanup goals and determining the magnitude of remediation efforts. • Allows estimation of total risk associated with the contaminant inventory.	• Does not provide spatial or temporal variability. • Fails to account for transport mechanisms and fate processes, limiting its utility for predictive modelling. • May overlook bioavailability and toxicity variations.
Mass Partitioning Analysis	• How are contaminants distributed among different environmental phases? • What is the relative contribution of each phase to overall contaminant mobility? • What site-specific factors (e.g. organic carbon, pH) influence contaminant partitioning? • Which environmental phase poses the greatest risk to receptors? • How does phase distribution inform remediation technology selection?	• Identify the distribution of contaminants across environmental phases (e.g. dissolved, sorbed, vapour). • Assess the bioavailability and mobility of contaminants. • Inform remediation technology selection based on phase-specific behaviour. • Predict vapour intrusion risks and indoor air impacts. • Evaluate the role of site-specific conditions (e.g. organic carbon, pH) on contaminant behaviour.	• Quantifies the distribution of contaminants across different environmental media (e.g. soil, water, air, and NAPL). • Helps identify key phases driving contaminant mobility and risk (e.g. sorbed vs. dissolved fractions). • Critical for understanding bioavailability	• Requires robust site characterization and high-quality data. • Can be highly sensitive to assumptions about partition coefficients (e.g. K_d, K_{ow}). • May oversimplify complex interactions, such as non-equilibrium or multi-phase partitioning.
Mass Flux and Mass Discharge	• How much contaminant mass is moving through the system over time? • What are the dominant transport pathways for contaminants? • How stable is the contaminant plume (e.g. stable, expanding, or contracting)? • How effective are current remediation efforts in reducing contaminant flux? • What is the impact of the contaminant flux on downgradient receptors?	• Quantify the rate of contaminant transport through a defined cross-sectional area. • Assess cumulative loading to stagnant water bodies or contaminant sinks. • Assess plume stability (e.g. stable, expanding, or contracting). • Evaluate the effectiveness of remediation efforts, such as pump-and-treat systems. • Identify the impact of contaminant flux on downgradient receptors, including drinking water wells or ecosystems. • Support regulatory compliance and decision-making by providing actionable metrics on contaminant movement.	• Quantifies the movement of contaminants through specific media or pathways (flux) and provides integrated measures of total contaminant movement (discharge). • Useful for evaluating ongoing source strength and for prioritizing source-area vs. plume-based remediation. • Allows comparison of contaminant transport rates across sites or within different zones at a site.	• Depending on specific method used, can be data-intensive and dependent on accurate hydraulic and contaminant concentration measurements. • May require installation of multiple monitoring points, increasing costs and complexity. • Cannot resolve detailed spatial variability without high-density data.
Mass Transfer Assessment	• How do contaminants move between environmental phases (e.g. soil to groundwater, groundwater to air)? • What are the rates of transfer processes, such as volatilization, sorption, or dissolution? • How does interphase mass transfer influence overall contaminant mobility and persistence? • Which transfer processes dominate under site-specific conditions? • How can mass transfer rates inform the design of targeted remediation technologies?	• Predict contaminant migration between environmental media (e.g. soil to groundwater or water to air). • Assess vapour intrusion risks for indoor air quality evaluations. • Inform the design of remediation technologies such as soil vapour extraction or in-situ chemical oxidation. • Evaluate the effectiveness of natural attenuation processes (e.g. biodegradation, volatilization). • Support fate and transport modelling by providing input on inter-phase contaminant dynamics.	• Helps quantify the rates at which contaminants move between different phases or media (e.g. volatilization, desorption, diffusion). • Useful for understanding and predicting natural attenuation processes and the effectiveness of remediation technologies. • Provides insights into rate-limiting steps for contaminant removal.	• Requires detailed site-specific data and may be computationally intensive. • Rate constants used are often generalized and may not account for site-specific heterogeneities. • Assumes equilibrium or steady-state conditions that may not reflect dynamic systems.

Method	Key Questions Answered	Key Applications	Advantages	Limitations
Mass Loading to Sensitive Receptors	• -What is the total contaminant mass entering or migrating through the system over a defined period? • What are the primary contributors to contaminant mass entering the system? • How does mass loading impact receptor risks, such as contamination of drinking water or ecosystems? • How effective are source control measures in reducing contaminant inputs? • How does mass loading compare to mass discharge in dynamic systems?	• Quantify the total contaminant mass reaching sensitive receptors, such as drinking water wells or surface water bodies. • Assess the potential human health and ecological risks posed by contaminant migration. • Evaluate the effectiveness of source control measures in reducing contaminant impacts. • Support regulatory compliance by demonstrating adherence to allowable contaminant load limits. • Inform remediation strategies to mitigate risks to sensitive receptors.	• Identifies the contribution of different sources or pathways to overall contamination levels. • Useful for pinpointing dominant contaminant sources or high-contribution areas. • Can guide resource allocation for remediation and monitoring.	• Assumes consistent loading rates, which may not hold in fluctuating environmental conditions. • Limited by uncertainty in source strength estimates and transport parameters. • Does not directly provide insights into contaminant fate or degradation.
Mass Balance Modelling	• What are the inputs, outputs, and transformations of contaminants within the system? • Are contaminant sources, sinks, and storage balanced? • How do natural attenuation processes or remediation efforts affect contaminant mass over time? • What is the long-term fate of contaminants under current site conditions? • How can the model predict contaminant behaviour and inform decision-making?	• Quantify contaminant inputs, outputs, and transformations within a defined system. • Assess the long-term fate and transport of contaminants across environmental media. • Evaluate the effectiveness of remediation strategies by tracking contaminant reductions. • Integrate multiple datasets (e.g. mass flux, mass partitioning) for comprehensive site assessment. • Identify data gaps and uncertainties in contaminant behaviour. • Support decision-making for site management and regulatory compliance.	• Provides a comprehensive framework for understanding contaminant inputs, outputs, and transformations within a defined system. • Supports predictive modelling and scenario analysis for remediation design and risk assessment. • Facilitates integration of multiple data types (e.g. chemical, hydrological, biological).	• Data-intensive and requires accurate input parameters for reliable results. • Complex systems may require simplifying assumptions, potentially limiting the model's accuracy. • Uncertainty in key parameters (e.g. reaction rates, degradation pathways) can propagate through the model, reducing confidence in predictions.

10.2 Data Requirements

The table below outlines the data requirements for various mass-based approaches used in contaminated site assessments. It compares the type of data needed, the level of data quality required, and the quantity of data necessary (e.g. number of samples, spatial and temporal coverage). These requirements vary depending on the complexity of each approach, as well as the specific environmental conditions and site-specific objectives. This comparison highlights the varying levels of effort and detail needed to implement these approaches effectively.

Table 10-2: Comparison of Data Requirements Between Mass Based Methods

Data Category	Total Mass of Contaminants	Mass Partitioning Analysis	Mass Flux / Discharge Quantification*	Mass Transfer Assessment	Mass Loading to Sensitive Receptors	Mass Balance Modelling
Contaminant Concentrations	Concentrations across media (soil, GW, SW, sediment, vapour); NAPL and porewater sampling.	Phase-specific concentrations (dissolved, sorbed, vapour); bioaccumulation data (BAFs, BCFs).	*Transect:* GW concentrations along transects. *Well Capture/Pumping:* Average concentration in pumped water. *Passive Flux Meters:* Mass sorbed on PFM sorbent. *Isocontours:* Interpolated concentrations from wells. *Solute Transport Models:* Initial/boundary concentrations from wells. *Thermal Tracer:* GW or mixed water concentration. *Isolation Flux:* Mass of VOCs. *Dynamic Flux:* VOC concentrations in exhaust gas.	Source/receptor and interface concentrations (dissolved, vapour, particulate).	Time-series concentrations in GW, SW, soil vapour, air; flux at interfaces.	Initial concentrations and flux measurements across transects.
Partitioning Coefficients	K_d, $K_{oc} \times f_{oc}$, Henry's Law, K_{nw} for phase distribution.	K_{oc}, K_d, K_{aw}, K_{ow}, K_{sa} for sorption and volatility.	*Passive Flux Meters:* Sorbent retardation factors. *Solute Transport Models:* Optional sorption coefficients.	Site-specific mass transfer coefficients for volatilization, interphase exchange.	Sorption/desorption coefficients for soil/sediment; attenuation rates.	Henry's Law, soil-water, sediment-water partitioning coefficients; retardation coefficients.
Physical Properties/Media Data	Soil/GW/SW/sediment/vapour: bulk density, porosity, moisture, f_{oc}, grain size; vadose zone thickness; temp (vapour pressure).	Soil (moisture, grain size); sediment (organic matter, clay); GW (hydraulic conductivity); vapour (depth).	*Transect:* Transect geometry. *Well Capture/Pumping:* Aquifer thickness. *Passive Flux Meters:* Well geometry (screen length, diameter). *Isocontours:* Plume cross-sectional area. *Solute Transport Models:* Porosity, dispersivity. *Thermal Tracer:* Spatial context of mixing zone. *Isolation Flux:* Area of chamber footprint. *Dynamic Flux:* Area of chamber footprint.	Soil (grain size, porosity, permeability); fluid properties (density, viscosity); tortuosity; geospatial data (topography, stratigraphy).	Vadose zone permeability, moisture; soil/sediment geochemistry (organic matter, CEC).	Hydraulic conductivity, porosity, dispersivity, diffusion coefficients; natural organic matter content.
Hydraulic/Geochemical Parameters	-	pH, redox, temp, DO, ionic strength, salinity affecting solubility/speciation.	*Transect:* hydraulic conductivity, hydraulic gradient. *Well Capture/Pumping:* Drawdown, transmissivity, storativity. *Passive Flux Meters:* Tracer loss for flux. *Isocontours:* Average hydraulic conductivity and hydraulic gradient. *Solute Transport Models:* hydraulic conductivity, hydraulic gradient, porosity, dispersivity. *Thermal Tracer:* Temperature.	Redox, pH, DO, electron acceptors, TOC; hydraulic conductivity, gradients.	Redox, pH, ionic strength in porewater/SW; hydraulic gradient, GW velocity.	Redox, pH, DO, major ions; GW velocity distribution, hydraulic conductivity, dispersivity.
Volume/Flow Data	Volume estimates (vadose zone, aquifer, SW body, sediment, NAPL zones); SW flow rate.	GW hydraulic conductivity; SW flow rates, dilution factors.	*Transect:* GW flux. *Well Capture/Pumping:* Pumping rate, capture zone. *Passive Flux Meters:* Deployment duration for flux calculation. *Isocontours:* GW flux. *Solute Transport Models:* Boundary conditions (heads/fluxes). *Thermal Tracer*: Optional total flow rate. *Isolation Flux:* Sampling duration. *Dynamic Flux:* Carrier gas flow rate.	GW velocities, flow rates, atmospheric conditions; no-flux zones.	GW flow rates, SW velocity/distribution, vapour flux, sediment resuspension rates; building-specific parameters (pressure, ventilation).	GW seepage velocities, precipitation/recharge, evapotranspiration, volatilization fluxes; vadose zone contributions.
Temporal/Spatial Variability	-	Seasonal/multi-depth sampling for dynamic trends.	*Transect*: Optional repeated measurements. *Well Capture/Pumping:* Multiple samples over time. *Isocontours:* Historical data for trends. *Isolation Flux:* Optional repreated measurements. *Dynamic Flux:* Real-time or periodic sampling.	Seasonal flow/temp fluctuations, spatial resolution of flow/turbulence.	Seasonal/transient concentration changes; meteorological data (wind, stability, deposition).	Seasonal/diurnal temp trends, recharge rates, time-variable source releases affecting transport/degradation.
Process-Specific Data	NAPL-specific (core sampling, fluorescence); vapour sampling.	Sorption/desorption isotherms, NAPL composition, colloidal fractions.	*Solute Transport Models:* Optional biodegradation rates; source mass, location, release rate. *Isolation Flux:* Retardation factors and sorption capacity of the passive sampling tube. *Dynamic Flux:* Carrier gas properties.	Advection, dispersion, volatilization, sorption, dissolution, biodegradation rates; diffusion paths.	Degradation, volatilization, biodegradation kinetics; dispersion patterns; airborne aerosol transport.	Degradation/transformation rates, reaction stoichiometry, source depletion rates.

Data Category	Total Mass of Contaminants	Mass Partitioning Analysis	Mass Flux / Discharge Quantification*	Mass Transfer Assessment	Mass Loading to Sensitive Receptors	Mass Balance Modelling
Collection Methods	Core sampling, fluorescence, soil gas sampling, porewater sampling.	Batch tests, core sampling, filtration, biota sampling, lysimeters, well tests, headspace sampling.	*Transect:* Wells, MLSs, direct-push, hydraulic tests. *Well Capture/Pumping:* Pumping wells, flow meters, observation wells. *Passive Flux Meters:* PFM installation, lab analysis. *Isocontours:* Existing wells, interpolation (e.g. kriging). *Solute Transport Models*: Field data, literature for calibration. *Thermal Tracer:* Temp sensors, GW sampling, stream gauging. *Isolation Flux:* Deployment and retrieval of chambers and passive sampling tubes. *Dynamic Flux:* Setup of chambers and real-time or periodic sampling.	Geophysical surveys, lab/field experiments (batch tests, column studies, tracer studies).	Monitoring wells, soil gas sampling, SW gauging, sediment sampling, air dispersion measurements.	Field measurements, lab-derived rates, literature values for model parameters.

10.3 Cost Analysis

The following table provides a comprehensive overview of the estimated costs associated with implementing various mass-based risk assessment methods at a standard oil and gas lease in Alberta, as defined in Section 1.3.1. These methods are priced to cover the acquisition of supplemental data specific to each approach, beyond a comprehensive CSM for soil and groundwater. Mass balance modelling is the most expensive approach ($52,500–$77,000), driven by its comprehensive approach, which necessitates extensive data collection on multiple processes and advanced modeling to track contaminant behaviour across the system. In contrast, the other methods fall within more moderate cost ranges, reflecting their varying needs for field data, lab analyses, and the complexity of evaluating contaminant dynamics in environmental media.

Table 10-3: Comparison of Cost Analysis Between Methods

Method	Estimated Cost Range	Description
Total Mass of Contaminants	$21,000 – $29,000	Quantifies the total amount of contaminants within the defined site area.
Mass Partitioning Analysis	$44,750 - $60,250	Assesses how contaminants distribute among phases (e.g. soil, water, air).
Mass Flux and Mass Discharge	$7,000 - $40,000	Measures contaminant movement and mass discharge rates through specific pathways. Cost ranges based on type of method used including transect methods, well capture/pump tests, passive flux meters, isocontours, and solute transport models.
Mass Transfer Assessment	$28,500 - $39,000	Evaluates the rates of mass transfer between environmental compartments.
Mass Loading to Sensitive Receptors	$30,750 - $41,000	Estimates the mass of contaminants reaching sensitive receptors (e.g. water bodies, ecosystems).
Mass Balance Modelling	$72,500 - $117,000	Balances inputs and outputs of contaminant mass within the system to understand fate and transport.

11. Conclusions and Next Steps

This report examines the application of mass-based methodologies for contaminated site management, with emphasis quantifying the mass of contaminants moving through or within a system, rather than relying solely on concentrations. These approaches were evaluated for their ability contribute to a holistic understanding of contaminant dynamics, accounting for transport, distribution, and interaction with environmental media. The report outlines how these methodologies can address challenges in site characterization, risk assessment, and remediation planning, providing practical tools for evaluating source zone strength, contaminant migration, and long-term stability. The current relationship of these methods to existing Alberta guidance and policy, gaps within Alberta guidance and opportunities for improvement were identified. Case studies and conceptual approaches were utilized to demonstrate the benefits of these methods compared to conventional concentration-based approaches, emphasizing their potential to improve decision-making for site management in Alberta.

12. Closure

We trust that this report satisfies your current requirements and provides suitable documentation for your records. A record of site conditions has been prepared and has been submitted in conjunction with this report. If you have any questions or require further details, please contact the undersigned at any time.

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Appendix A. Mass Partitioning as a Tool for Assessing PCB Behaviour and Risks in the Hudson River Superfund Site

Appendix A.
Case Study: Mass Partitioning as a Tool for Assessing PCB Behaviour and Risks in the Hudson River Superfund Site

A.1 Introduction

The Hudson River PCBs Superfund Site (the “site”) is a large and complex environmental remediation project stretching approximately 200 miles (321 kilometers) from Hudson Falls to New York Harbor. The site became heavily contaminated with polychlorinated biphenyls (PCBs) due to industrial discharges by General Electric (GE) facilities in Fort Edward and Hudson Falls. Between 1947 and 1977, an estimated 1.3 million pounds (589,670 kilograms) of PCBs were released into the Hudson River (the “river”). These contaminants, used in electrical equipment manufacturing, are highly toxic, bioaccumulative, and persistent in the environment (TAMS Consultants et al. 1997).

In 1984, the United States Environmental Protection Agency (USEPA) classified the Hudson River as a Superfund site under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA; TAMS Consultants et al. 1997). This designation was due to the widespread contamination of sediments, water, and biota, posing significant risks to human health and the environment. The remediation efforts required a comprehensive understanding of PCB behaviour, transport, and fate within the river system—a challenge addressed using mass partitioning analyses integrated into various assessments.

This case study examines the application of mass partitioning in the assessment of the Hudson River PCBs Superfund Site, providing insights into the behaviour, transport, and risks of PCBs across environmental media and receptors to evaluate the effectiveness of various remedial scenarios.

A.2 Applications of Mass Partitioning

A.2.1 Data Used

The assessment of PCB contamination in the Hudson River relied on a comprehensive dataset to examine partitioning between sediments and the water column, transport dynamics, bioavailability, and contamination sources. Data collection included chemical, physical, and biological measurements to characterize PCB behavior and its ecological impact. Key datasets included sediment and porewater PCB concentrations, organic carbon content, geochemical properties, hydrodynamic data, and PCB concentrations in surface water and groundwater. These measurements supported modeling efforts to quantify PCB distribution, transport, and bioaccumulation within the river system. The primary data sources are summarized below:

- Contaminant concentrations in site media: PCB concentrations in groundwater, surface water, porewater, sediment, and suspended solids (including dissolved, particulate-bound, and total fractions), integrating suspended solids data to determine PCB association with particulates.

- Total organic carbon (TOC) and dissolved organic carbon (DOC): quantified to assess organic matter's influence on PCB partitioning and bioaccumulation, including octanol-water partition coefficient (K_{ow}) data.
- Grain size distribution and percent solids: used to characterize sediment properties and their influence on PCB sorption.
- Hydrodynamic data: river flow, velocity, and turbulence parameters to evaluate PCB transport dynamics.
- Geochemical and physical-chemical parameters: pH, redox potential, temperature, annual sediment concentrations, and monthly water concentrations to assess PCB release mechanisms and distribution across compartments.
- Fish tissue PCB concentrations: measured for bioaccumulation modeling, including lipid-normalized concentrations.
- Historical monitoring data: long-term datasets on fish weight, lipid content, and feeding preferences.
- Environmental concentrations: sediment and freely dissolved water PCB concentrations, integrating multi-year hindcasting from fate and transport models with site media measurements.
- Food web data: dietary compositions of fish species based on gut content analyses and feeding behavior studies.
- Background PCB levels in reference sediments, surface water, and groundwater: used to differentiate site-related contamination from regional background.

A.2.2 Sediment-Water Partitioning

Mass partitioning between sediments and the water column was used to evaluate PCB mobility and bioavailability within the Upper Hudson River study area, encompassing 40 miles of the river from Fort Edward to Troy, New York. Sediment-water partitioning was characterized using site-specific organic carbon partition coefficients (K_{oc}), which quantify the equilibrium distribution of PCBs between sediment organic carbon and the aqueous phase (TAMS Consultants et al. 1997 and 2000a). The relationship is expressed as:

$$K_{OC} = \frac{C_s}{C_d * f_{OC}}$$

where:

- K_{oc} represent site-specific organic carbon partition coefficient (L/kg);
- C_s represents PCB concentrations in sediment (mg/kg);
- C_d represents dissolved PCB concentrations in porewater (mg/L); and
- f_{OC} is the fraction of organic carbon in the sediment (unitless).

This relationship was used to estimate porewater concentrations and understand desorption processes during resuspension events. High K_{OC} values indicated strong affinity for sediment-bound organic matter, while lower values reflected greater potential for desorption into porewater. Measurements in the Hudson River demonstrated elevated PCB levels in porewater near contamination hot spots, such as the Thompson Island Pool, where historical contamination was higher (TAMS Consultants et al. 1997 and 2000a). As more PCBs desorb into porewater, their

bioavailability to aquatic biota increases, leading to greater bioaccumulation in predatory species and potential human exposure.

A.2.3 Groundwater-Surface Water Interactions

Groundwater discharge was a known pathway introducing PCBs to surface water in the Hudson River. Studies confirmed that groundwater migrated through bedrock fractures from the GE Hudson Falls site and that some capped but unlined dredge spoil areas discharged groundwater directly to the river (TAMS Consultants et al. 1997 and 2000a). Recognizing this, partitioning dynamics governing PCB transport from sediments and porewater into groundwater and surface water were investigated to understand the mechanism of how PCBs move between media. Three-phase partitioning models were applied to show the diffusion of PCBs into groundwater and their subsequent discharge to surface water.

In a two-phase partitioning model, the sorbate is considered either in the particulate fraction or the water fraction, which includes both truly dissolved sorbate and sorbate bound to dissolved or non-filterable organic matter. In contrast, three-phase models separately account for sorbate bound to dissolved organic matter, offering a more detailed understanding of PCB movement and bioavailability (TAMS Consultants et al. 1997 and 2000a). As such, the utilized three-phase models accounted for their association with particulate organic carbon (POC), dissolved organic carbon (DOC), and the truly dissolved phase[1] of PCB in water. The total PCB concentration (C_T) in the water column was expressed as:

$$C_T = C_d(1 + K_{DOC} * DOC + * K_{POC} * POC)$$

where:

- C_T is the total PCB concentration in the water column (µg/L);
- C_d is the truly dissolved PCB concentration (µg/L);
- K_{DOC} and K_{POC} are the partition coefficients for DOC and POC (unitless);
- DOC and POC represent their respective concentrations (mg/L).

This framework provided a more comprehensive understanding of PCB behaviour, particularly for lower molecular weight congeners, which exhibited greater binding to DOC compared to higher molecular weight congeners that preferentially partitioned to suspended solids and sediments. These relationships were used to quantify PCB flux from groundwater to surface water, clarifying that while porewater diffusion and advection contributed to PCB movement from sediment into the water column, groundwater discharge was a persistent source of PBCs to surface water. This analysis identified significant contributions from high-DOC groundwater and porewater, highlighting the role of these media as a persistent PCB source to surface water (TAMS Consultants et al. 1997 and 2000a).

A.2.4 Bioavailability and Food Web Modeling

Mass partitioning was used to understanding PCB bioavailability and its impact on the food web within the Hudson River. The FISHRAND model utilized porewater PCB concentrations and

[1] "Truly dissolved phase" refers to the fraction of a contaminant that exists in water in a freely dissolved state, excluding portions bound to dissolved organic matter, colloids, or suspended particulates. This distinction is important in bioaccumulation modelling, as the truly dissolved fraction represents the most bioavailable form for uptake by aquatic organisms.

sediment-water partitioning coefficients to predict PCB uptake in fish through both waterborne and dietary exposure pathways (TAMS Consultants et al. 2000b,c,d). PCB concentrations in fish tissue (C_{fish}), expressed as:

$$C_{fish} = BCF * C_d$$

where:

- C_{fish} represents the concentration of PCBs in fish tissue (ng/g lipid weight or ng/g wet weight)
- BCF is the bioconcentration factor (L/g), and
- C_d is the dissolved PCB concentration in water (ng/L).

This approach allowed for the estimation of bioaccumulation and the trophic transfer of PCBs to piscivorous wildlife and humans. Model predictions were validated by comparing estimated fish tissue PCB concentrations with measured values from monitoring programs, ensuring alignment between predicted and observed contamination levels. By modelling these pathways and verifying accuracy with empirical tissue data, the assessment quantified risks from fish consumption, a major exposure route for human populations relying on the river for subsistence fishing (TAMS Consultants et al. 2000b,d).

A.2.5 Fate and Transport Modeling

Two-phase and three-phase equilibrium partitioning models were used to quantify the partitioning of PCBs between dissolved, particulate-bound, and organic matter-bound phases in sediment and water. These partitioning models underpinned the HUDTOX (Hudson River Toxic Chemical Model) fate and transport model, which simulated PCB flux between sediment, water, and organic carbon. By incorporating equilibrium partitioning, HUDTOX predicted the long-term distribution and downstream transport of PCBs. These projections offered insights into the effectiveness of various remedial strategies and their potential to lower PCB loading throughout the river system over time (TAMS Consultants et al. 2000c).

A.2.6 Risk Assessment and Exposure Pathways

Mass partitioning results fed directly into the calculation of exposure point concentrations (EPCs) for both human and ecological receptors. EPCs were derived from modeled PCB concentrations in sediment, water, and biota, incorporating variability in partitioning behaviour across the site. These concentrations informed risk estimates for ingestion, dermal contact, and inhalation pathways, with a particular focus on fish consumption as a dominant exposure route for humans. The calculated risks guided remediation goals and cleanup levels, to reduce risks to human health and ecological receptors to tolerable levels (TAMS Consultants et al. 2000c,d).

A.2.7 Background and Source Differentiation

Partitioning dynamics were also applied to differentiate PCB contamination attributable to site-related sources from background levels. This was achieved by comparing observed sediment and water PCB concentrations with natural and anthropogenic background data from upstream and reference locations. Models such as HUDTOX incorporated site-specific partitioning coefficients to identify “hot spots” of contamination linked to historical discharges, distinguishing them from diffuse regional sources. This analysis helped prioritize areas for targeted remediation and allowed for consideration of natural attenuation processes in risk assessments (TAMS Consultants et al. 1997 and 2000a).

A.3 Conclusion

Mass partitioning was an important component of the Hudson River PCBs Superfund Site assessments, providing insights into the transport, bioavailability, and risks associated with PCB contamination. By integrating partitioning data into sediment-water interactions, food web modeling, and transport simulations, the USEPA and its partners developed effective strategies for remediation and risk reduction. The comprehensive application of mass partitioning underscores its importance in addressing complex environmental contamination challenges.

A.4 References

TAMS Consultants, Inc., The CADMUS Group, Inc., and Gradient Corporation. 1997. Phase 2 Report: Data Evaluation and Interpretation Report, Hudson River PCBs Reassessment Remedial Investigation / Feasibility Study, Volume 2C. Prepared for the U.S. Environmental Protection Agency and the U.S. Army Corps of Engineers. February 1997.

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[2] Remedial Investigation / Feasibility Study

Appendix B. Case Study: Mass Flux and Weight of Evidence Approaches in Assessing Aquatic Impacts of a Release of Molybdenum Containing Water

Appendix B.
Case Study: Mass Flux and Weight of Evidence Approaches in Assessing Aquatic Impacts of a Release of Molybdenum Containing Water

B.1 Introduction

In southeast Alberta, an incident resulted in the release of water containing a molybdenum additive into the surrounding environment. The released water flowed across a grazed pasture ultimately reaching a fish-bearing creek approximately 215 meters downslope from the release point, and damaging vegetation along its flow path. At the time of the release, the creek had a wetted width of 1.1 m to 3.3 m, with a water depth ranging from 0.05 m to 0.35 m over a 600 m stretch. Emergency response teams intervened, using HydroVac trucks and graders to construct interception trenches to prevent further contamination. Approximately 590 m^3 of the molybdenum containing water was released, affecting an area of approximately 3,856 m^2 within an agricultural field (pasture). Several environmental activities were carried out to assess the impacts of the release, including soil sampling along the flow path, surface water sampling along the creek, opportunistic groundwater sampling at the base of a remedial excavation, fish habitat assessments, and acute lethality tests of impacted release water and nearby surface water. Cleanup efforts included removing 90 m^3 of molybdenum contaminated soils and installation of erosion controls. The incident was investigated and reported to appropriate regulators.

Although the project was multifaceted, addressing both terrestrial and aquatic environmental impacts, this case study focuses on evaluation of impacts to the aquatic environment through a mass-based approach. Specifically, this case study highlights the application of Water Quality Based Effluent Limits (WQBEL), a mass flux-based methodology, used to determine the toxicity of the spill discharged into the nearby creek. WQBEL calculations, which incorporate pollutant concentration, flow rate, and the receiving water's dilution capacity, were a critical line of evidence (LOE) integrated into a broader Weight of Evidence (WOE) framework. Using mass balance equations, WQBEL predicted the resultant instream toxicity of pollutants in toxicity units (TUs), providing quantitative insights into potential risks to aquatic life in the receiving waterbody.

B.2 Methodology and Results

Risks to aquatic life in the receiving surface waterbody were assessed using several LOEs that were amalgamated using a WOE approach with the objective of developing a unified conclusion regarding the probability and magnitude of harm (Canadian Council of Ministers of the Environment [CCME] 2020). These LOEs included surface water chemistry; comparison of fish habitat in the exposure areas to background (upstream) areas, and toxicity tests to rainbow trout (*Oncorhynchus mykiss*) and *Daphnia magna*. An overview of the methodology and results for each of these LOEs, along with a summary of the associated WOE analysis, are described below.

B.2.1 Surface Water Chemistry

Surface water samples were collected at 13 locations during three sampling events in the summer of 2022, conducted within 24 hours, 11 days, and 22 days after the release. Sample locations included one sample from the water storage tank, one sample from the release point (source), and 11 samples from the receiving environment. The creek samples consisted of two upstream samples and nine downstream samples during each sampling event. The samples were analyzed for ammonia (from the sulphur expansion tank only), routine potability, and both dissolved and total metals.

Concentrations of cadmium and molybdenum in water from the water storage tank exceeded Environmental Quality Guidelines for Alberta Surface Waters (Government of Alberta [GoA] 2018), and concentrations of various metals (arsenic, cadmium, chromium, iron, manganese, molybdenum, silver, and zinc) were also found in the released water at the source above surface water guidelines. Surface water sampling in the creek conducted 12 hours after the release showed concentrations of metals like aluminum, iron, and molybdenum in downstream samples slightly elevated above upstream samples, but below surface water guidelines. Subsequent sampling 11 and 22 days after the release revealed sporadic exceedances of guidelines, particularly for dissolved iron and total silver, but concentrations returned to below detection limits in later samples. Overall, the concentrations of iron and molybdenum showed a downward trend and, with the removal of impacted soils, concentrations and surface water quality were expected to return to baseline levels.

B.2.2 Fish Habitat Assessment

The receiving creek was assessed using a small watercourse habitat classification system to evaluate aquatic conditions and fish habitat. The fish habitat assessment covered an area from approximately 100 m upstream to 500 m downstream of the release point and was completed two and 28 days after the release. The fish habitat assessment measured various habitat parameters, including water depth, substrate composition, and field measurements of water quality (i.e. temperature, dissolved oxygen, conductivity, and pH); and provided a quality rating for the entire assessed reach. A follow-up visit found no new sediment deposition, increased algal growth, and observed fish in good condition with no signs of stress or mortality. Follow-up visits confirmed that field measurements of water quality remained consistent across the reach during both fish habitat assessment periods.

B.2.3 Toxicity Testing and Water Quality Based Effluent Limits

Given discharge to the creek was temporary, toxicity tests for two species — rainbow trout and *Daphnia magna* — were conducted using source water from the release point to determine the acute lethality of the released solution. Results from these tests included:

Rainbow Trout LC50 Test: The 96-hour lethal concentration (LC50) exceeded 100% vol/vol, indicating dilution of source water from the creek would result in less than the LC50 endpoint for fish.

Daphnia Magna LC50 Test: The 48-hour LC50 was measured at 33% vol/vol, suggesting potential impacts to aquatic invertebrates from the source water entering the creek.

These results were interpreted using methods outlined in the WQBEL Procedures Manual (Alberta Environmental Protection 2015) to predict the resultant instream toxicity after effluent mixing with creek water. Results from toxicity tests were used to calculate acute toxicity units (TU_a) as the inverse of the sample endpoint solution concentration (Equation 1).

$$Acute\ Toxic\ Unit = TU_a = \frac{100}{LC_{50}}$$ Equation [1]

Where:

LC_{50} = concentration (expressed as percent dilution) of effluent that is lethal to 50% of test organisms (% dilution).

The TU_a results are as follows:

Rainbow Trout: Since the LC50 exceeded 100% vol/vol, it was assumed the instream effluent concentration would meet the negligible effects criteria protective of fish (i.e. $TU_a < 0.3$).

Daphnia Magna: 3.03 for the source solution.

TU_a, along with stream flow measurements and predicted potential effluent volume that discharged into the creek were then used calculate the resultant instream toxicity using the mass balance equation outlined in the WQBEL Procedure Manual (Equation 2).

$$C_{r,t} = \frac{Q_e C_{e,t} + Q_s C_{s,t}}{Q_e + Q_s}$$ Equation [2]

Where,

Q_e = volume of effluent discharge (m^3/s);

Q_s = volume of receiving water body available for mixing(m^3/s);

$C_{e,t}$ = effluent toxicity (unitless);

$C_{s,t}$ = upstream toxicity (unitless);

$C_{r,t}$ = resultant instream toxicity of substance after mixing (unitless); and

The values used for each input parameter is discussed below.

Volume of Effluent (Q_e) and Volume of receiving water body available for mixing (Q_s)

The volume of effluent (Q_e) was estimated to be 0.0042 m^3/s, using the following assumptions:

- Approximately 594 m^3 of source solution was released;
- Approximately 90 m^3 of the source material (including impacted soil and water) was removed from site for off-site disposal[1];
- The worst-case release duration was approximately 33 hours and 4 minutes, which does not account for two interception trenches installed at approximately 30 minutes and 1 hour post-release to mitigate overland flow.
- Release rate was linear/uniform.

[1] The volume estimate includes the disposal of five truckloads, each carrying approximately 12 m^3 of source material, along with an additional truck manifest indicating the disposal of 30 m^3 of source material.

See calculation below.

$$Total\ Volume\ Released = 594\ m^3 - 90\ m^3$$

$$= 504 m^3$$

$$Release\ Flow\ Rate = \left(\frac{504\ m^3}{119040\ s}\right)$$

$$= 0.0042\ m^3/s$$

The flow rate of receiving water body (Q_s) was measured to be 0.12 m^3/s.

Effluent Toxicity ($C_{e,t}$)

Inputs for effluent toxicity are the TU_a values calculated for rainbow trout (TU_a < 0.3) and *Daphnia magna* (TU_a = 3.03).

Upstream Toxicity ($C_{s,t}$)

The upstream toxicity is assumed be in pristine conditions and a value of 0 was used for TU_a as outlined by the United States Environmental Protection Agency (USEPA; 2010).

Resultant Instream Toxicity ($C_{r,t}$)

The predicted instream effluent toxicity for *Daphnia magna* was calculated to be $C_{r,t\text{-}daphnia}$ = 0.79. This resultant instream toxicity, expressed as a TU_a, was compared to negligible risk criteria for instream toxicity of effluent after mixing, which is 0.3 TU_a for acute scenarios (Alberta Environmental Protection 2015). Since the resultant instream toxicity exceeds this threshold, there is a reasonable potential for adverse effects, indicating a risk of exceeding acceptable toxicity levels in the receiving water.

B.2.4 Weight of Evidence Analysis

A WOE framework was applied to integrate findings from the creek's surface water chemical analyses, the fish habitat assessment, and toxicity tests using source water. The approach involved integrating measurement endpoints linked to the LOEs to evaluate the likelihood and magnitude of ecological risk. A preliminary assessment of the relative merit of each LOE was conducted, followed by an evaluation of the magnitude of response for each. These analyses were combined to reach an overall conclusion regarding the effect of the release on the aquatic environment in receiving creek.

Surface water chemistry results showed negligible risk, as measured concentrations of constituents in surface water samples collected from the creek were below Alberta's surface water guidelines (GoA 2018). The fish habitat assessment found no significant changes downstream compared to upstream conditions, with no observable impacts to habitat quality or aquatic life. Toxicity testing using source water on rainbow trout indicated no risk, while testing on *Daphnia magna* revealed a temporary exceedance of toxicity thresholds, suggesting moderate short-term risk. As such, the WOE analysis concluded the risk to aquatic life was low to negligible due to:

- Limited duration of elevated toxicity;
- Declining contaminant concentrations over time; and
- Absence of observable stress or mortality in aquatic species during assessments.

B.3 Conclusions

The assessment of the water containing a molybdenum additive demonstrated the effectiveness of combining WQBEL and a WOE approach to evaluate impacts to the aquatic receiving environment. The release of approximately 590 m^3 of molybdenum-treated water temporarily impacted the receiving creek, with toxicity testing indicating a short-lived exceedance of acceptable thresholds for *Daphnia magna*. However, surface water chemistry analyses showed contaminant concentrations in the creek declining over time to below guidelines, while fish habitat assessments confirmed no significant differences in habitat quality or aquatic life upstream and downstream of the release, with no observed fish mortality. This case study highlights the importance of mass-based methodologies like WQBEL in effectively assessing the short-term and localized risks of effluent releases, while confirming the long-term recovery and resilience of the aquatic environment through declining contaminant levels and unaltered fish habitat.

B.4 References

Alberta Environmental Protection. 2015. Water Quality Based Effluent Limits Procedures Manual. December 1995.

CCME (Canadian Council of Ministers of the Environment). 2020. Ecological Risk Assessment Guidance Document. PN 1585 ISBN 978-1-77202-044-1 PDF.

Government of Alberta (GoA). 2018. Environmental Quality Guidelines for Alberta Surface Waters. March 2018.

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Appendix C. Empirical Mass Balance Modelling to Quantify Contaminant Sources in the Lower Passaic River

Appendix C.
Case Study: Empirical Mass Balance Modelling to Quantify Contaminant Sources in the Lower Passaic River

C.1 Introduction

The Lower Passaic River (LPR) is an Operable Unit (OU) of the Diamond Alkali Superfund Site in Newark, New Jersey that was established in response to significant environmental contamination caused by numerous industrial and municipal sources. Beginning in the late 19th century, manufactured gas plants, paper mills, petroleum refineries, and chemical manufacturers discharged wastewater directly into the LPR as the industrial hubs of Newark and Paterson grew. Over 100 industrial facilities, contributed to the pollution. A significant source of contamination was the Diamond Alkali Company's facility, which, between 1951 and 1969, produced a defoliant chemical known as "Agent Orange", which contains dioxin, as well as other substances. The manufacturing processes at this facility resulted in byproducts that were released directly into the LPR (Louis Berger Group Inc [LBG] 2014a,b).

The LPR is the focus of intense remediation planning due to the accumulation of toxic pollutants in its sediments, including dioxins and furans, polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), metals, and pesticides. To better understand the fate and transport of these contaminants, an Empirical Mass Balance (EMB) model was developed (LBG 2014a,b).

C.2 Methodology

The EMB model was designed to quantify the contributions of tributaries, Second River and stormwater outfalls (SWOs) / combined sewer overflows (CSOs), Newark Bay, and the Upper Passaic River as contaminant sources compared to the resuspension of legacy sediments and their associated contaminants. Ultimately understanding the sources of contaminants through EMB modeling was used to provide insights for evaluating remedial alternatives.

The EMB is a receptor-type chemical mass balance model that uses Beryllium-7 (Be-7)-bearing sediments as a tracer to identify the contributions of contaminants from various sources. Be-7 is a naturally occurring, particle-reactive radioisotope with a half-life of approximately 53 days that serves as a marker for recently deposited sediments (LBG 2014a). Its short half-life allows for sediments deposited within the last six to 12 months to be analysed, integrating inputs from external sources and internal river processes, including resuspension, mixing, and deposition dynamics, prior to deposition. Specifically, The EMB model quantifies the mass contributions of contaminants from the following key sources (Figure C-1):

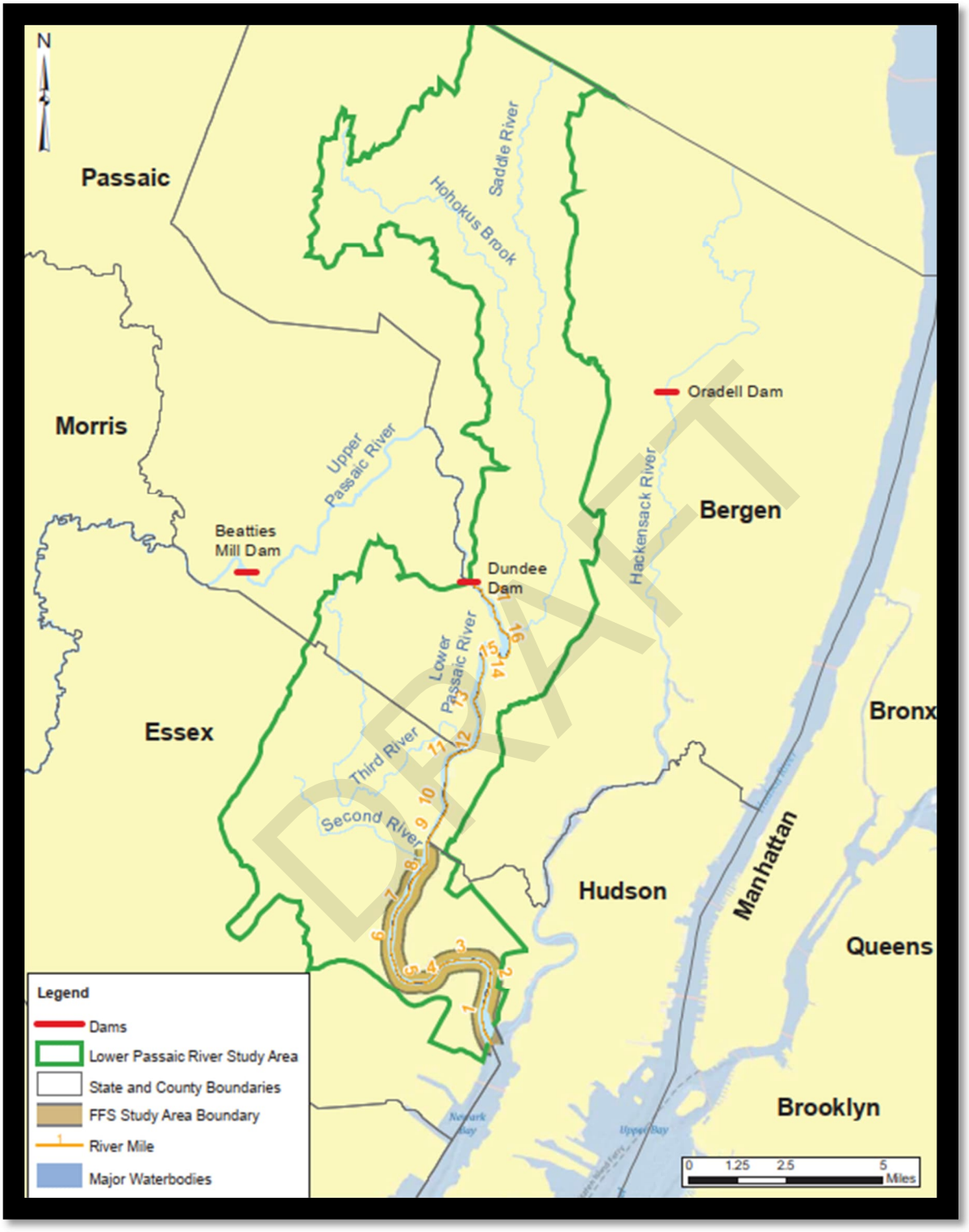

Figure C-1: Site Area. Republished from: LBG 2014b.

1. Upper Passaic River (above Dundee Dam);
2. Newark Bay;

3. Saddle River;
4. Third River;
5. Second River and the SWOs;
6. Combined Sewer Overflows (CSOs); and
7. Resuspension of legacy sediments within the LPR (LBG 2014a).

This approach allows the model to account for both contemporary inputs and the persistent impact of legacy pollution.

The foundational equation for the EMB model represents the contaminant concentration in the receptor sediments as a linear combination of the contributions from identified sources. Mathematically, the contaminant concentration in the surface sediments of the LPR, $C_{surface,i}$ for a given contaminant *i*, is described as:

$$C_{surface,i} = \frac{1}{S_{total}} \sum_{j=1}^{p} M_{i,j}$$

Where:

$M_{i,j}$ = the mass of contaminant *i* contributed by source *j*;

S_{total} = total sediment mass deposited in the LPR;

p = number of sources contributing to the receptor sediments;

j = index representing each individual source contributing to the contaminant mass in the surface sediments; and

i = indexes the different contaminants present in the sediment.

This receptor-type contaminant mass balance model, where the receptor is defined as recently deposited Be-7-bearing sediments, calculates the total contaminant mass as the cumulative contributions from various external and internal sources, reflecting the integrated loads influencing the LPR. For a fixed number of sources, the receptor (i.e. recently deposited, Be-7-bearing sediments) observation of the i^{th} contaminant is modeled as a linear combination of sources' contaminant species, presented as:

$$Y_i = \sum_{j=1}^{p} f_j * C_{i,j} + \epsilon_i$$

Where:

Y_i = receptor concentration for the i^{th} contaminant concentration

f_j= fraction of solids contributed by the j^{th} source to the receptor

C_{ij} = the i^{th} contaminant concentration for the j^{th} source

ϵ_i= error associated with the concentration of the i^{th} contaminant

p= number of sources contributing to the receptor sediments

j = index representing each individual source contributing to the contaminant mass in the surface sediments

i = indexes the different contaminants present in the sediment.

The equations derived by substituting the identified variables into the main equation were solved simultaneously using a least squares method to estimate the fraction of the contaminant burden (i.e. contaminant flux) contributed by each source to the LPR. The EMB model incorporated a total of 22 parameters, with 13 used directly for model optimization and the remaining nine for further model evaluation. The EMB model's input data includes contaminant concentrations for metals (chromium, copper, lead, mercury), organic contaminants (PCBs, PAHs, pesticides), and normalizers (iron, total organic carbon [TOC]) (LBG 2014a). Sampling primarily focused on surface sediments (0-15 centimeters), targeting recently deposited material. The model accounted for resuspension, porewater exchange, and bioturbation as key processes influencing sediment contamination. While sediment was the primary medium analysed, water column suspended solids were also examined in certain contexts (e.g. CSO and SWO contributions) (LBG 2014a).

The EMB model calculations utilized Microsoft Excel® Solver alongside the Crystal Ball® 7 add-on (Decisioneering, Denver, CO, USA), a tool commonly used for optimization problems. The model produced a best estimate solution[1] derived from average source and receptor concentrations. Monte Carlo analysis was then conducted to evaluate variability and uncertainty in the model; and sensitivity analyses were performed to examine how SWO concentrations and the model's solids constraint influenced the best estimate solution. Historical trends were assessed using dated sediment cores and comparisons between past and recent sampling efforts (LBG 2014a).

C.3 Results

The EMB Model analysis highlighted sediment resuspension as the predominant contributor to the contaminant burden in recently deposited sediments of the LPR. Resuspension accounted for 28 to 65% of the recently deposited solids, with a best estimate of 48%. The following table summarizes the estimated contributions of external sources and resuspended contaminants to newly deposited sediments in the LPR, as determined through EMB model analysis.

[1] "Best estimate solution" was based on average input values, representing the most probable outcome from the mass balance modelling. It was refined through a Monte Carlo analysis (10,000 iterations) to assess uncertainty and used to project contaminant trajectories with percentile ranges.

Table C-1: Sources and Contributions of Contaminants to Newly Deposited Sediments in the Lower Passaic River

Source Category	Description	Contribution to Recently Deposited Sediments (%) (Range)	Best Estimate (%)
Internal Sources (Sediment Resuspension) - *Remobilization of legacy sediments and associated contaminants already present within the LPR system.*			
Resuspension (Solids)	Legacy sediments remobilized from the LPR riverbed and reintroduced into recently deposited sediments.	28 - 65	48
2,3,7,8-TCDD (Resuspension)	Legacy 2,3,7,8-TCDD remobilized from contaminated sediments in the LPR riverbed and reintroduced into newly deposited sediments.	87 - 100	97
Total PCBs (Resuspension)	Legacy PCBs remobilized from contaminated sediments in the LPR riverbed and reintroduced into newly deposited sediments.	59 - 90	81
4,4'-DDE (Resuspension)	Legacy 4,4'-DDE remobilized from contaminated sediments in the LPR riverbed and reintroduced into newly deposited sediments.	52 - 88	78
PAHs (Resuspension)	Legacy PAHs remobilized from contaminated sediments in the LPR riverbed and reintroduced into newly deposited sediments.	17 - 58	39
Heavy Metals (Resuspension)	Legacy heavy metals (copper, chromium, mercury, lead) remobilized from contaminated sediments in the LPR riverbed and reintroduced into newly deposited sediments.	-	-
External Sources (Waterborne Transport) - *Total solids and associated contaminants transported from external locations (Upper Passaic River, Newark Bay, and Other Sources) to the LPR.*			
Upper Passaic River	Solids and associated contaminants transported from the Upper Passaic River to the LPR.	13 - 49	32
Newark Bay	Tidal exchange contributions bringing solids and associated contaminants transported from Newark Bay to the LPR.	<1 - 44	14
Other Sources (Combined)	Includes tributaries, SWOs, and CSOs, with relatively small contributions of solids and contaminants to the LPR.	2 - 12	N/A
Contaminant Contributions from External Sources - *Originate from external waterborne sources above (i.e. Upper Passaic River, Newark Bay, and the other sources combined).*			
Total PCBs from Upper Passaic River	PCBs transported from the Upper Passaic River to the LPR.	4 - 22	11
Total PCBs from Newark Bay	PCBs transported from Newark Bay to the LPR.	<1 - 25	7
PAHs from Upper Passaic River	PAHs transported from the Upper Passaic River to the LPR.	24 - 70	47-53*
PAHs from Newark Bay	PAHs transported from Newark Bay to the LPR.	<1 - 30	6
4,4'-DDE from Upper Passaic River	4,4'-DDE transported from the Upper Passaic River to the LPR.	21-Apr	10
4,4'-DDE from Newark Bay	4,4'-DDE transported from Newark Bay to the LPR.	<1 - 34	8
PAHs from Other Sources	PAHs transported from tributaries, SWOs, and CSOs to the LPR.	<1 - 17	-
4,4'-DDE from Other Sources	4,4'-DDE transported from tributaries, SWOs, and CSOs to the LPR.	1 - 10	4

* PAH contributions from the Upper Passaic River vary depending on specific compounds: 53% for benzo[a]pyrene (range 27 - 70%) and 47% for fluoranthene (range 24 - 64%).

Overall, the EMB Model identifies sediment resuspension as a significant source of contaminants, particularly 2,3,7,8-TCDD, underscoring the importance of legacy sediments as a critical driver of the LPR's contaminant burden (LBG 2014a). This analysis informed remedial actions, leading to a combination of dredging and capping strategies to mitigate contaminant flux. Removal actions targeted the most contaminated sediments near the former Diamond Alkali facility, while engineered caps were designed to isolate contaminants, reduce resuspension, and stabilize sediments in high-risk areas (LBG 2014b). These efforts aimed to minimize exposure risks, prevent further downstream transport, and enhance long-term recovery of the river ecosystem (LBG 2014a).

C.4 Conclusions

The results of the EMB model emphasize the continued influence of legacy sediments as the primary source of contamination in the LPR. While contemporary inputs from tributaries, CSOs, and Newark Bay contribute to the system, they are overshadowed by the significant burden of historical pollution stored within the sediments. These findings highlight the importance of remediation strategies that mitigate sediment resuspension and reduce in-situ contaminant loads to achieve meaningful reductions in pollutant levels in the LPR.

C.5 References

Louis Berger Group Inc (LBG). 2014a. Appendix C: Mass Balance Modeling Analysis. In Remedial Investigation Report for the Focused Feasibility Study of the Lower Eight Miles of the Lower Passaic River. Prepared for the U.S. Environmental Protection Agency

Louis Berger Group Inc (LBG). 2014b. Remedial Investigation Report for the Focused Feasibility Study of the Lower Eight Miles of the Lower Passaic River. Prepared for the U.S. Environmental Protection Agency.