Many regulatory discussions about sites with groundwater contamination are driven by point-in- time measurements of contaminant concentration—snapshots of contaminant concentrations that may appear to be relatively stable or to show notable changes over time. However, concentration data alone cannot answer all questions critical to contaminant plume assessment or management. Among these questions are the following:

- Is the current distribution of contaminants stable, expanding, or contracting?
- How will a proposed remedial action affect the future distribution, transport, and/or fate of contaminants?
- What will be the risks and exposures at various points of potential exposure throughout the foreseeable future?
- How much source removal will be needed before transitioning to other technologies such as in situ bioremediation or allowing monitored natural attenuation (MNA) to complete the site remediation?
- Which hydrogeologic zones should be targeted by remedial action for maximum benefit?
- What are the options for optimizing existing remedial actions to reduce life cycle costs?

The answers to these questions require an understanding of plume dynamics and specifically the mass flux and mass

discharge of contaminants within the plume. Mass flux (expressed as mass/time/area, e.g., $g \cdot d^{-1} \cdot m^{-2}$) and mass discharge (expressed as mass/time, e.g., g/d) can provide important information about source strength, natural attenuation rates, and possibly the areas of the subsurface through which the majority of the mobile contaminant mass is moving (assuming sufficiently high vertical resolution). The terms "total mass flux" or "integrated mass flux" are used by some authors; both refer to the sum of all of the individual mass flux estimates across an entire plume, which this document terms "mass discharge." In this overview, we use the terms "mass flux" (J) and "mass discharge" (M_d).

Nothing in this technology overview on the use and measurement of mass flux and mass discharge supersedes existing regulatory requirements from state or federal agencies. As always, familiarity with state, federal, and local environmental rules is necessary before proceeding with any environmental investigation.

Environmental regulatory standards for contaminants in water do not consider mass flux; they consider only concentrations of contaminants in groundwater in terms of mass per volume. This focus on concentration is understandable since aqueous contaminant concentration is used to determine and regulate the risk to a given receptor exposed to the groundwater at a specific location. This regulatory approach causes site managers to focus primarily on the concentration trends through time and space, relying on data from specific monitoring wells to manage plume remediation or to document performance and compliance. Because mass flux is not needed for concentration-based plume management and additional data must be collected for its calculation, managers typically have not calculated, evaluated, or fully appreciated the value of mass flux for site management.

Over time, recognition of the benefits of mass flux estimates has grown, as a series of quotations shows. First, academic specialists identified a potential application:

Therefore, the ultimate impact of plumes emanating from solvent DNAPL source zones can be evaluated in terms of impact of relatively small annual mass fluxes to the receptor such as water-supply wells or surface waters. In some cases, the fluxes present significant risk to human health and/or the environment, and extensive remedial action is warranted. In other cases, the fluxes are insignificant, and remedial action would provide little or no actual environmental risk reduction." (Pankow and Cherry 1996)

Then, the U.S. Environmental Protection Agency (USEPA 1998) summarized three key reasons for developing mass flux or discharge estimates (here, the word "flux" refers to mass discharge as defined in this document):

1. The reduction in the flux [discharge] along the flow path is the best estimate of natural attenuation of the plume as a whole.

2. The flux [discharge] is the best estimate of the amount of contaminant leaving the source area. This information would be needed to scale an active remedy if necessary.

3. The flux [discharge] estimate across the boundary to a receptor is the best estimate of loading to a receptor."

Next, the complementary values of both mass flux and concentration data in assessment and remediation were recognized:

In summary, measurements of mass flux of the contaminants and footprint parameters— not just concentrations—are necessary to document cause-and-effect and to assess long- term sustainability/permanence. Site-characterization and

monitoring plans should be proactively designed to accommodate mass flux estimates. (USEPA 2001a)"

Mass flux is now being used more frequently to characterize and monitor groundwater contamination (USEPA 2003) due to a growing recognition that mass flux data can provide a more complete measure of the exposure posed by the contaminants than static point concentration estimates alone (Einarson and Mackay 2001; Buscheck, Nijhawan, and O'Reilly 2003). Intense interest in developing and testing better methods to measure and estimate mass flux began when it was identified as one of the most pressing research needs for management of chlorinated solvent sites (SERDP 2004; Einarson, 2017; Annable, 2019; CRC Care, 2016). Recent improvements in mass flux measurement have made the development of sufficiently detailed estimates more practical and economical.

While it is unlikely that mass flux will globally replace point concentrations as the metric for regulatory compliance, it is a powerful tool for developing remedial goals and defining decision points. Mass flux and mass discharge information help managers better understand the impact of a complex plume on the environment and/or receptors, as well as better evaluate the impacts of treatment and whether interim remedial objectives have been achieved. The decision to collect and evaluate mass flux data is site specific. It should consider the reliability of other available data, the uncertainty associated with mass flux estimates, the specific application(s) of the mass

flux data, and the cost-benefit of collecting mass flux data. Figure 1-1 helps illustrate the application of mass flux and mass discharge in the site investigation and remediation process.



Figure 1-1. Mass flux and mass discharge application within the remedial process. (Numbers preceding applications correspond to those in Table 1-1.)

Mass flux estimates can better characterize a contaminated site than typical monitoring networks (Feenstra, Cherry, and Parker 1996). Typical monitoring plans focus primarily on defining plume boundaries and concentration trends, but chemical concentrations (and groundwater velocities) vary tremendously across a plume, and areas of significant flux may be missed during source and extent delineation. A mass flux calculation requires measurement of the variability in concentrations and

velocities within a plane of the plume and therefore is based on a more thorough site characterization. Additionally, mass flux values at different times and places along a plume show the combined impact of all of the physical, chemical, and biological processes acting on the contaminants. The additional understanding of plume dynamics provided by mass flux improves the conceptual site model (CSM), which helps site managers make better remediation decisions (Nichols and Roth 2004, Basu et al. 2006). Prior ITRC documents also have concluded that the addition of mass flux data can result in more credible remediation decisions than concentration data alone (ITRC 2004, 2008a, 2008b). Specifically, mass flux information can improve the understanding and management of contaminated sites several ways:

- Mass flux estimates along transects near source zones can yield critical information about source zone strength, source zone architecture, and the degree of heterogeneity in the aquifer.
- Mass discharge estimates can improve assessment of the potential exposure to a receptor, such as a water supply well or surface water body.
- Mass flux data comparisons over time and space can directly measure the attenuation capacity of the aquifer, delineate the highest contaminant mass and mass flux zones within a plume, and identify the optimal treatment zones within a plume.
- Mass discharge and mass flux estimates can be used to develop remedial goals and performance metrics, select and design remediation systems, monitor remedy performance, and define transition points, in time or space, between technologies.
- Mass discharge can help regulatory agencies and site managers prioritize remediation of multiple sites based on differences in source strength and threats to receptors.

The use of mass flux and mass discharge is increasing and will accelerate as field methods improve and practitioners and regulators become more familiar with their application, advantages, and limitations.

Mass flux characterization is intended to reduce uncertainty, and a cost-benefit analysis should be undertaken before beginning such a characterization. For example, when using mass flux estimates to size a remediation effort, questions such as "How wrong can this estimate be without compromising effectiveness or protectiveness?" should determine the scope and resolution of the mass flux definition. Further, it must be realized that mass flux characterization can increase total project costs without a concomitant rise in data usability.

As with any investigation, integration of mass flux or discharge evaluations into decision making begins with the questions to be answered and the goals to be reached. The mass flux/discharge calculation must directly address these questions and the remedial objectives. Data use during a decision-making process should be defined. To help managers optimize mass flux or mass discharge data collection, Table 1-1 lists remedial objectives (as identified in Figure 1-1), decision points, and the relative data density needed to achieve each. The data density column is intended only to provide a relative frame of reference and to make the point that different objectives require different data, not to specifically recommend the quantity of data to be gathered. For instance, estimating residual source strength may require relatively fewer data points if the objective is to evaluate source strength reduction during and after treatment. However, if you want to understand heterogeneity in contaminant mass flux across the vertical transect to design a more efficient treatment or you want to estimate the natural attenuation capacity of a plume using multiple transects, then data density requirements increase. Additional detail on each application is found in later sections of this document as referenced in the fourth column.

Table 1-1. Summary of mass flux data and decision points for contaminant plume remediation and management

Remedial applications	Mass flux data use	Flux-informed decision points	Relevant document section	Relative data density of mass flux or mass discharge
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1. Determine whether you need to treat contamination to achieve remedial goals or MNA is appropriate	Estimate source strength	Is the mass discharge from the source area sufficiently high (for instance, greater than the natural attenuation capacity in the plume) to necessitate active treatment?	3.1	Low
	Estimate contaminant plume stability	Is the trend in contaminant mass flux or discharge throughout the plume indicative of an expanding or contracting plume?	3.1.1	High if using multiple plume transects
	Estimate the balance between the mobile contaminant mass and the natural attenuation capacity of a plume	Is the natural attenuation capacity (estimated from the reduction in contaminant mass discharge measured at a series of transects oriented perpendicular to the plume axis) sufficiently high to achieve remedial action objectives? Or is active treatment required in the source area and/or plume?	3.1.1	Medium to high if using multiple plume transects
2. Evaluate risk to groundwater receptor(s)	Estimate risks and exposures to groundwater receptors over time at various points of potential exposure	Does mass discharge to a receptor location necessitate active treatment of the source area or dissolved-phase plume?	3.2	Low to medium
3. Evaluate remedial alternatives: select appropriate technology or suite of technologies to achieve remedial goals	Determine remedial action objectives to achieve remedial goals	What is the reduction in mass discharge from a source area or across a plume transect needed to achieve remedial goals?	3.3.1	Low to high depending on system design and treatment volume(s)
	Determine appropriate remedial technology or technologies for source and/or plume treatment	What technologies are capable of achieving the required reduction in mass flux or discharge from a source area or across a plume transect?	3.3.2	
Develop and optimize remedial design	Evaluate heterogeneities in source zone architecture	What is the minimum treatment volume or mass required to achieve remedial action objectives?	3.3.3	High
	Estimate source strength reductions necessary to transition technologies (i.e., to in situ bioremediation or MNA)	Has source strength (i.e., discharge) been reduced sufficiently to transition to less-aggressive treatment?	3.3.3	Low
	Estimate distribution of contaminants relative to transmissive zones	What is the optimal treatment configuration to achieve remedial action objectives?	3.3.3	High

4. Evaluate remedial performance	Determine whether treatment efficiencies are sufficient to achieve remedial goals • Compare mass removal for a remediation system to mass discharge estimate • Compare total electron acceptor demand to mass discharge of electron acceptors	Is treatment achieving mass flux or discharge remedial action objectives and ultimately remedial goals?	3.4	Low to high depending on system design and treatment volume(s)
5. Evaluate compliance and long-term monitoring	Determine contaminant mass discharge or flux limits to achieve remedial goals	Is the remedial system achieving the desired mass flux and/or discharge objectives deemed acceptable for achieving remedial goals?	3.5	Low to medium
6. Site prioritization	Determine mass loading from the source or to a receptor	Measure mass discharge along a transect perpendicular to flow • At the downgradient edge of the source zone • Just upgradient of a potential receptor Compare source strength and potential impacts to receptors among sites to assess resource allocation	3.6	Low to medium

In summary, this technology overview describes the concepts and practice of mass flux and mass discharge to foster the appropriate uses of these tools. Section 2 describes the basic principles of mass flux and mass discharge measurement. Section 3 describes current and potential applications. Section 4 describes methods of estimating mass flux and mass discharge in groundwater, specific models and tool kits, and factors that can affect distributions and estimates. Finally, Sections 5 and 6 summarize specific barriers or challenges associated with mass flux and mass discharge approaches and corresponding research needs.

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