Mass Balances

Conservation of mass is foundational to the building of models of environmental engineering systems. It applies to all systems at all scales with the exception of systems involving nuclear reactions.

To build a mass balance for a system requires a clear definition of the system being considered. A system model requires a clear definition of the system to work. In chemical systems, this is referred to as the system's *CONTROL VOLUME*. A control volume defines the boundary of the system, it defines what is inside and what is outside the system and it defines which movements cross the system boundary. It is common practice, and often a best practice, to communicate your system's defined control volume using a diagram. The diagram is kept simple but it clearly captures what is INSIDE the control volume and what is OUTSIDE. It also clearly identifies all of the means of mass exchange between the inside and outside.

Equation **1** provides the most general form of the mass balance equation.

$$Mass In - Mass Out = Mass Accumulation \qquad Equation 1$$

The *Mass IN* is the mass that is moving across the control volume boundary into the system (control volume). The *Mass OUT* is the opposite. The *Mass ACCUMULATION* is the net change in mass within the control volume.

Equation **1** is simple and powerful. It is equally applicable to the scale of the entire Earth and the scale of a microbial cell. It is applicable over the time period of a millennium, over a nanosecond and as an instantaneous rate. The equation applies to ALL mass movement, to chemical compound movement and to each chemical element's movement. The application to chemical compounds requires the appropriate inclusion of chemical reactions, as chemical compounds are NOT conserved entities. Developing the ability to apply a mass balance in all of these contexts requires practice and experience.

Applying a mass balance over a finite period of time leads to Equation **2**.

$$Mass In - Mass Out = \Delta Mass$$

Equation 2
Mass In - Mass Out = Mass_{final} - Mass_{initial}

Where *Mass In* in this case is the total mass entering the control volume over the entire time period of interest. *Mass Out* is the same but represents the total mass leaving. The Δ

Mass is the net change of mass inside the control volume over the time period. It is the final mass minus the initial mass. Each term has mass dimensions.

Equation **3** provides the form of the mass balance for instantaneous rates. The word "rate" frequently is dropped because it is understood to be present when the accumulation is provided as a derivative. In this case, the dimension of each term is mass per time.

Rate Mass In – Rate Mass Out =
$$\frac{dM}{dt}$$

Mass In – Mass Out = $\frac{dM}{dt}$
Equation 3

Gases, liquids and solids move across boundaries as a result of gradients. Often total pressure gradients drive bulk gas and liquid motion. Thus fluid mechanic principles drive this bulk movement. Individual compounds may move across the boundary as a result of their own concentration gradients (mass transfer principles) and / or by active transport carrying compounds within the bulk phase movement. Imagine a conveyor belt delivering apples into a control volume. This bulk apple movement certainly brings apples into the control volume but it also brings any pesticide found in the apples.

Table 1 provides a few expressions for defining mass and mass flow rates when the mass is not directly available or provided. Total volume (V) and total volumetric flows (Q) are often more readily accessible. The density (ρ) in this case is the total bulk density. The total density is the summation of all of the individual compound concentrations (C_i).

Table 1:	Mass	Expressions
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	Mass	Mass Rate
Total	V ho	Qρ
Component i	V C _i	$Q C_i$

Equation **1**, Equation **2**, and Equation **3** all apply to mass balances on total (as an aggregate of all compounds in the systems) and on each element. It applies to individual compounds in a non-reactive setting. For reacting settings, the mass balance equations are modified to explicitly address the reaction process.

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Mass In – Mass Out + Generation – Consumption
$$= \frac{dM}{dt}$$
 Equation 4

The net result of all generation and consumption terms must be zero when Equation **4** is summed across all of the compounds in the system. The handling of the generation and consumption terms depends on the nature of the reaction taking place. Options include: stoichiometry, equilibrium and reaction kinetics.

Stoichiometry option is associated with the assumption that reactions are going to completion. The reactants are consumed while the products are generated. The stoichiometric coefficients create the relationships between compounds and lead to the coupled connections between each compound's version of Equation **4**. Not all of the reactants will be consumed if the reactants are not entering the system in the stoichiometric ratio.

The equilibrium option is associated with the assumption that the reactions are able to reach equilibrium within the system. An equilibrium coefficient (K_p) provides the relationships between compounds and leads to coupled equations.

The reaction kinetic option is associated with a situation in which the reactions are too slow to reach completion or equilibrium. Reaction kinetics is described with rate laws. A rate law, in standard form, describes consumption or generation term per unit volume as a function of compounds in the system. Compound mass balances become coupled when the rate law depends on multiple compounds.