**Partition Coefficients:**

***Definition:***

*The ratio of concentrations of a compound in the phases of a mixture of two “immiscible” solvents (or phases) at equilibrium.*

**Figure 1:** When two phases such as octanol and water are side by side, a molecule has a choice to move into either one. In this case molecules that do not “like” water (it takes too much energy for them to be there) will prefer the octanol. Other molecules that “like” water and are water “soluble” will prefer the water and not the octanol. ***“like dissolves like”***

There are many examples in nature where partition coefficients are used. They are particularly important when we try to determine how dangerous a chemical may be to humans. We can use partition coefficients to figure out how much of a chemical will stick to us once we drink it, breathe it or come into contact with it (sunscreens, waterproof coating on clothing, fabric softeners).

Examples of systems:

* Air/water
* Sediment water
* oysters/water
* Octanol /water
* EVA/water
* Fatty tissue/water

Examples of compounds:

* Pharmacueticals
* Pesticides
* Herbicides
* Oil
* Plastics
* Flame retardants
* Combustion products

We will use partition coefficients to help us understand how so much of a chemical can store up in one phase like our fatty tissue when its concentrations in water or even the food we eat are MUCH lower,

**The tools we need:**

We need to understand how to get a partition coefficient. First you put your two phases, we’ll call them P and M, together so they are in contact. Then you add your chemical. You need to know how much P, M (mass or volume) you have as well as how much chemical you are adding. Once you have this set up you let your “system” reach a balance where the chemical stops shifting (though the molecules never stop moving), Once this happens you have “equilibrium”, Equilibrium is defined as a “closed” system (you cap off the system so the phases and chemical do not have anywhere else to go) where the concentrations of the chemical in each phase does not change over time. You can then take a sample of each phase and measure the chemical concentration in it, Cp and CM (in units of mass or moles per liter or mass or moles per gram). The ratio of these two concentrations gives you your partition coefficient. It’s that simple and VERY powerful,

**Experiment:**

Ever wonder why we are not suppose to eat too much fish? Ever wondered what bioaccumulation is really about? Let’s make a surrogate “you” and surrogate “source” of chemicals and see what happens. As a surrogate living organism we can use something organic like vegetable oil and we can use water as an environmental source. A convenient way to place the two side by side is using a separatory funnel because it allows us to see the two phases (oil/water). We will use different dyes that can be seen to represent different chemicals and will determine the partition constants for three different compounds. The compounds will be chosen such that one “likes” water (hydrophilic) and one “likes” oil (hydrophobic) and another that is in between.

**Purpose:** To determine partition coefficients for three compounds in an oil/water system.

**Apparatus:** 3 separatory funnels (500 ml), stand, clamps, 300 ml oil, 300 ml water and three chemical dyes. (conventional food coloring, Nile red (NIL) andf Pinacyanol chloride (PCYN) or fabric dyes).

Dye to each funnel, swirl and let sit. Sample both fluids by absorption and determine the concentration in each using a calibration curve. Determine the partition coefficient.

**Resources:**

Abbey Dyes - <http://www.abbeycolor.com/solvent-dyes.php>

**Additional components:**

* Add the chemical to one of the phases and monitor the uptake in the second until equilibrium is reached.
* Add co-solvents
* Change phases
* Change temperature