In environmental chemistry we want to know:

- the (equilibrium) concentration of pollutants in various environmental phases in order to compare them to toxic thresholds.
- the mass of a pollutant in various phases in equilibrium. E.g. we want to calculate how much of a solvent is needed to extract 95% of a given pollutant out of a 1 litre water sample.
- the fractions of a chemical in various phases in equilibrium. E.g. if in a soil, only 10 % of a chemical resides in the aqueous phase and 90% are sorbed to the soil matrix, then the transport velocity of this chemical with the water will be 10 times slower than for the water itself. In other words the chemical is retained by a factor 10.

All this information can be calculated based on the respective partition constant and some additional information:

In the script the following formula is derived for the fraction of chemical *i* that resides in phase 2 in a two-phase system in equilibrium.

$$f_{i2} = \frac{1}{1 + K_{i12}\frac{V_1}{V_2}}$$

V_1 and V_2 are the volumes of the two phases and $K_{i\,12}$ is the respective partition constant expressed in volumetric concentrations.