

## Quantitative equilibrium calculations

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# Spreadsheet

Under the following link [Mehr-Phasensystem.xls](#) you can access a spreadsheet which allows you to do the following calculations:

**Sheet A:** Calculate equilibrium concentrations and mass fractions of a chemical in any two-phase system (e.g. water-air) where volumetric units are used. Required input data (green cells) are the air-water partition constant and the volumes of both phases.

**Sheet B:** Calculate equilibrium concentrations and mass fractions of a chemical in any three-phase system (e.g. water-air-org. phase) where volumetric units are used. Required input data (green cells) are the air-water partition constant, the org. phase-water partition constant and the volumes of all phases.

**Sheet C:** Similar to Sheet B but the concentration in the organic phase is normalized to the **mass of carbon** of the organic phase (instead of the volume of the complete organic matter). Consequently the amount of organic phase is also expressed as mass of organic carbon. This setting is typically used for soil systems. Therefore the input actually asks for the mass of the solid soil material and that fraction of it which is comprised of organic carbon.

**Sheet D:** Similar to Sheet C but with (mineral) surfaces as additional sorbing phase.

