Chemical Speciation (CS), as defined by IUPAC, is the “distribution of an element amongst defined chemical species in a system”.

Since the chemical and physical properties of any elements of compounds are strictly related to the species in which they occur in particular conditions, CS studies are of outmost importance to evaluate their impact, activity and/or performances in real systems of environmental, biological and technological/industrial interest.

One of the most effective ways to perform Speciation Analysis is through computer modelling based on thermodynamic equilibrium data (mainly, but not only, stability constants). To this aim, reliable sets of formation constants are necessary to evaluate the network of the most relevant interactions between all components of the system under investigation.

Considering that several real systems (e.g., seawater, estuarine and fresh waters, biological fluids, process and/or waste waters) are, from a chemical point of view, multielectrolyte aqueous solutions in which many elements and compounds are simultaneously present in a wide range of conditions, it is evident how CS studies of these systems represent a particularly challenging task.

Starting from the basic concepts regarding the chemical speciation of real aqueous systems, lessons will then focus on: i) the evaluation of the most critical aspects related to the experimental determination of thermodynamic parameters in multicomponent aqueous solutions; ii) their modelling as a function of chemical and physical variables like composition, ionic strength and temperature; iii) the use of computer tools and calculation approaches for data elaboration and speciation analysis; iv) examples and applications of speciation studies.