L02. Advances in hard-modelling of chemical processes

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Hard-modelling of chemical processes is a neglected area in the field of chemometrics. While soft-modelling methods are powerful and the only option in many applications, hard-modelling is significantly more robust and importantly provides useful quantitative information such as rate or equilibrium constants. For that reason, it is much more commonly used by the wider community of chemists.

Hard-modelling consists of determining the appropriate chemical model that describes the process under investigation, together with the determination of the optimal values for a set of parameters defined by that chemical model. Several crucial aspects of hard-modelling that have been addressed in the recent past will be introduced and discussed in this presentation:

- For multivariate data potentially a very large number of parameters have to be fitted; in such instances, methods that differentiate between linear and non-linear parameters are absolutely crucial
- The determination of the correct model (chemical process) is often not easy and thus time consuming. Genetic algorithms can help.
- Many chemical processes are complex and their parameters cannot be determined from one single experiment; global analysis of many individual experiments taken under different conditions is the solution.
- Traditional chemical experimentation is done under strictly controlled conditions: thermostating to control temperature, buffering to control pH, and inert salts to control ionic strength; it is possible to allow changes in these conditions during the experiment by accommodating them into the computation. This can significantly experimental design.

The application of the above principles will be demonstrated using appropriate chemical systems. In particular, reference will be made to our present research which is directed towards the investigation of the chemistry of CO_2 in aqueous solution, particularly in the presence of organic amines. This research is relevant for PCC (Post Combustion Capture), the attempt of removing CO_2 from the exhaust gases of fossil fuel based power production. It could be a significant contribution to the abatement of the greenhouse effect.