# Mechanistic Chemistry Studies: From Instrumental Design and Insitu Detection to Suitable Methods for Reaction Modelling.

Sebastien Cap, Yorck-Michael Neuhold, Tamas A. Godany, Konrad Hungerbühler

ETH Zurich, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich, Switzerland
sebastien.cap@chem.ethz.ch

Detailed mechanistic studies of complex chemical reactions are challenging. They require state of the art in situ instrumentation, a well-defined reaction environment, powerful chemometric methods to elucidate the kinetics and thermodynamics, and chemical intuition.

Kinetic and thermodynamic analysis are well established under quasi-ideal conditions, e.g. for dilute homogeneous systems [1]. However, in contemporary synthetic chemistry, highly concentrated (solvent-free) conditions are often encountered, or heterogeneity can be present as for example in crystallisation/dissolution reactions. Then, kinetic/mechanistic analysis generally becomes very complex.

We have developed a new high performance reaction calorimeter offering a well characterised, versatile and highly controlled reaction environment suitable to study chemical systems of such complexity [2]. In this contribution, we present our studies on a four step consecutive reaction including preceding reactant dissolution. Deterministic model development based on mass transfer and time evolution of the dissolving solid particles are discussed. Novel methods to elucidate the evolution of the particle size distribution from in situ laser reflectance, ATR-IR measurements and heat release during the course of the reaction will be presented.

Financial support by the Swiss National Science Foundation (grant no 200021-113473) is gratefully acknowledged.

[1] Maeder M., Neuhold Y.-M., Puxty G., King P., Phys. Chem. Chem. Phys., 2003, Vol 5, 2836.
[2] Puxty G., Fischer, U., Jecklin M., Hungerbuhler K., Chimia, 2006, Vol 60, 605.