Data Analysis in CombiCat

Ph.D. student: **Susana C. Cruz**   **email:** cruz@science.uva.nl

Supervisors: **Johan A. Westerhuis, Gadi Rothenberg**

Promoters: **Age K. Smilde, Alfred Bliek**

Research group: **PAC, HKCP**

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Concept

Combinatorial catalysis (CombiCat) is a new field that brings together rational catalyst design and High Throughput Experimentation (HTE). Much effort has been focused on new methods for the synthesis and screening of catalyst libraries using novel techniques. However, these new methods must go hand-in-hand with **Data Analysis** development, because the amount of data generated in combicat systems is LARGE.

This is especially true when optimisation and kinetic studies are concerned, since catalytic efficiency often depends on reaction conditions (pressure, temperature, pH, *etc.*) as well as on catalyst composition.

What we measure

Spectroscopic data

What we want
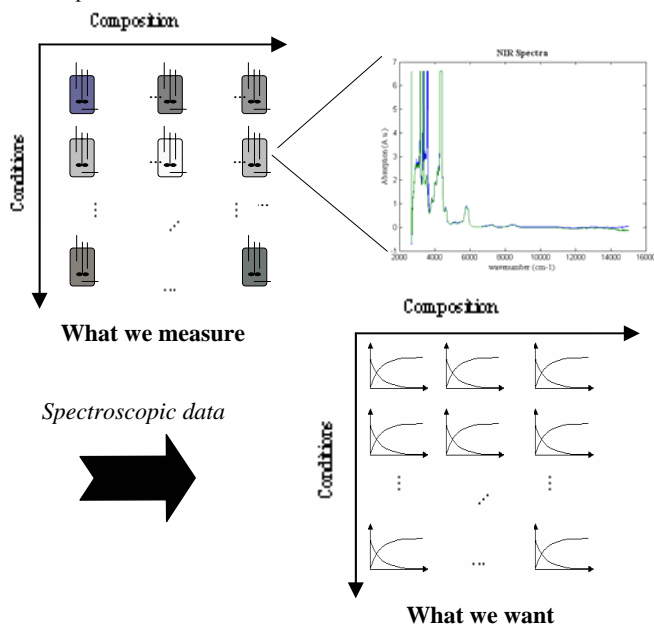
♦ **Multiblock Data Analysis**

We are developing chemometric methods that combine the data of **all** the experiments to improve the estimation of kinetic profiles.
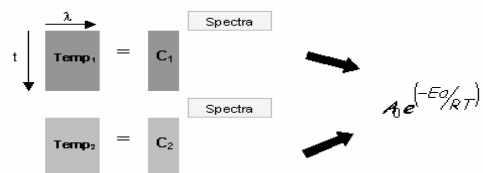

♦ **Spectroscopy not chromatography**

HTE systems perform well when coupled to real-time analysis. In this case, spectroscopy has some key advantages over GC and HPLC:

- It is faster (every ~5 seconds);
- It is non-invasive and non-destructive;
- Sample preparation is easier;
- Multiplexing.

First Results

The fast Heck coupling between iodobenzene and *n*-butyl acrylate catalysed by a bulky monodentate phosphoamidite complex was chosen as a suitable test case. Reaction progress was observed using FT-NIR and results were analysed with the Net Analyte Signal (NAS) approach.

Analyte signal

$$C_{NBA}(t) = C(0) \cdot e^{(-kt)}$$

$$k_{obs} = 0.055 \pm 0.004 \ min^{-1}$$
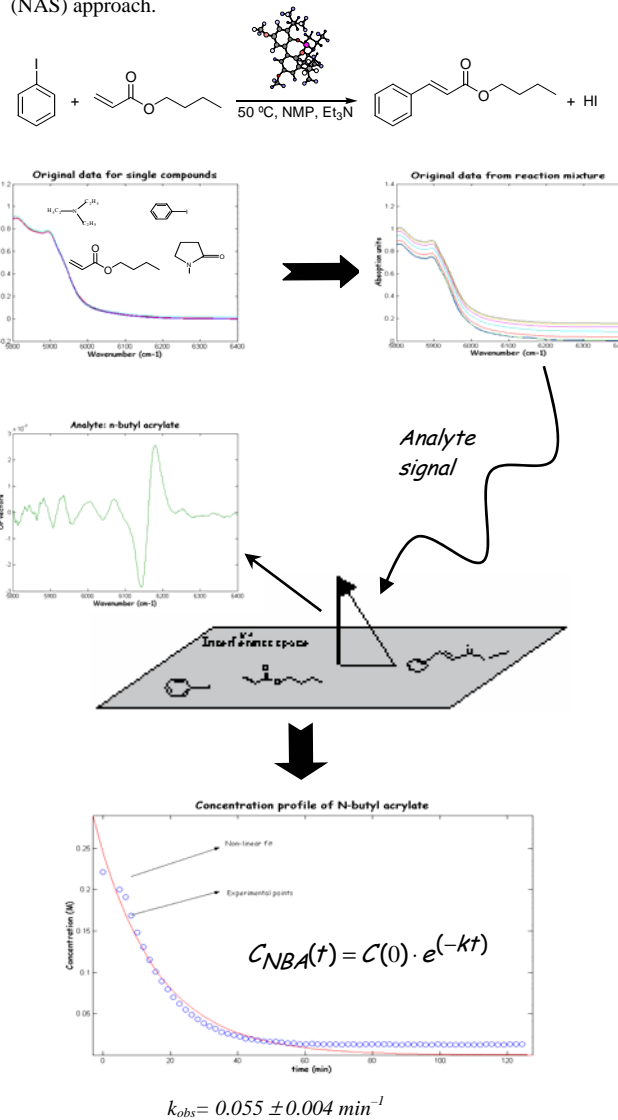
What next?

Derive activation energy values from the experimental data and compare our results with GC. Explore the possibilities of Raman to obtain additional chemical information.