

# Data Analysis in CombiCat

Susana C. Cruz, Petra J. Aarnoutse, Gadi Rothenberg, Johan A. Westerhuis, Age K. Smilde and Alfred Bliek  
Department of Chemical Engineering, University of Amsterdam, The Netherlands.

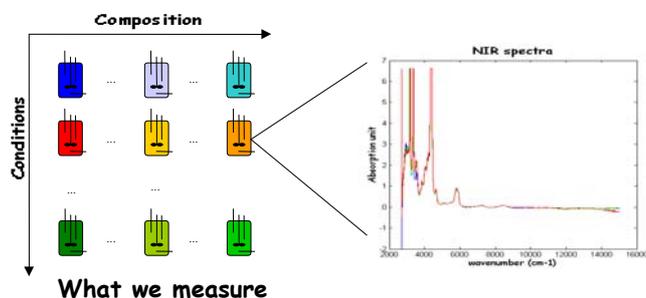


cruz@science.uva.nl

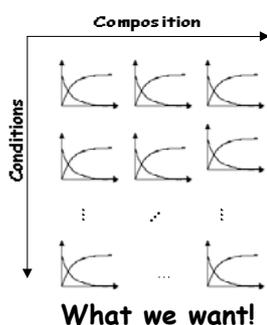
## Concept

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**<sup>1</sup>.

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.

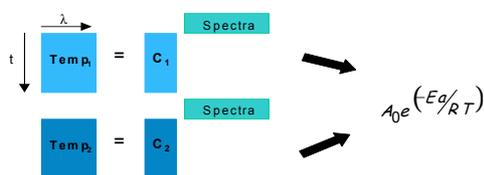


Spectroscopic data



## ◆ Multiblock Data Analysis

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



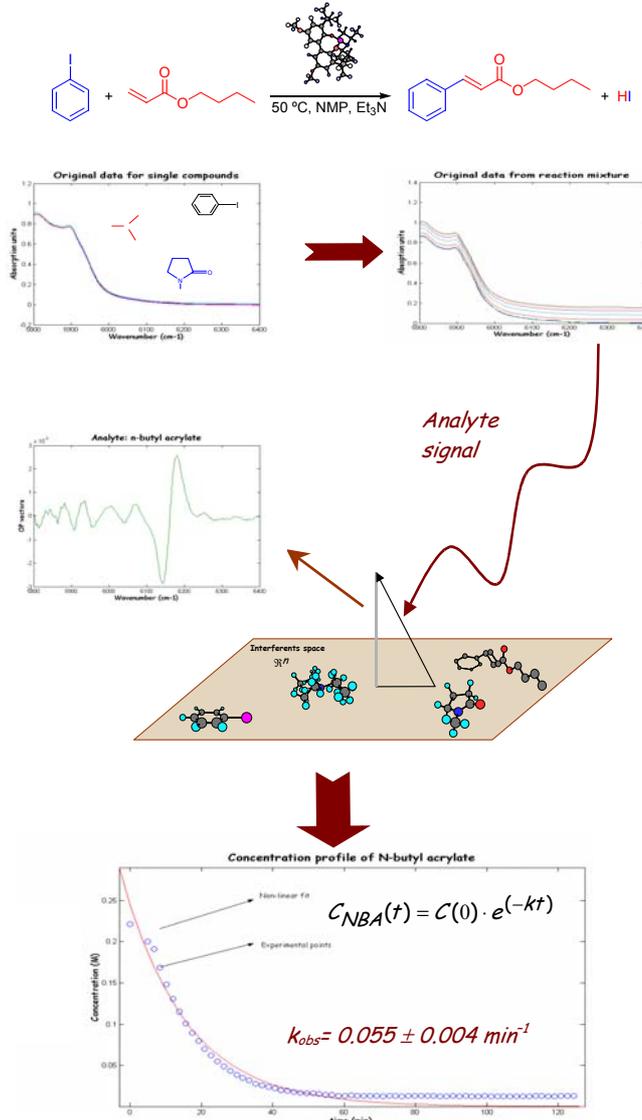
## ◆ Spectroscopy not chromatography

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 phosphoramidite complex<sup>2</sup> 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.



## What next?

Derive activation energy values from the experimental data and explore the possibility of using Raman to obtain the same type of results.

\* We thank Gino van Strijdonck and Maarten Boele for a generous gift of this catalyst complex.

1. See for example J. Scheidtmann, P. A. Weiss and W. F. Maier, *Appl. Catal. A*, **2001**, 222, 79.

2. G. P. F. van Strijdonck, M. D. K. Boele, P. C. J. Kamer, J. G. de Vries and P. W. N. M. van Leeuwen, *Eur. J. Inorg. Chem.*, **1999**, 1073.