

Reaction Monitoring with in situ infrared spectroscopy (FTIR-ATR)

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In thermoanalytical investigations the determination of the composition of the reactive solutions and the evolved gases is very important, especially when monitoring reactions with instable intermediates. In situ spectroscopy such as online FTIR, where the light is guided by silver halide fibers from the spectrometer to the ATR probe tip ^(1, 2), is a very useful tool to monitor several parameters: e.g. rate of reaction, endpoint determination, semibatch optimization by controlling feed using in situ information of the reactive analyte.

In this contribution two examples will be presented to gain an insight of the advantages of this online molecular video during the reactions:

- 1) Grignard reaction: online monitoring of halogenides and calculating kinetic relevant parameters of this exothermic reaction may give a lot of information to settle security relevant issues for scale up topics to define production parameters.
- 2) Fermentation: semibatch reaction which uses online spectroscopic information to control feed is very important in PAT/QbD issues.

The potential of online monitoring of different characteristic wavelengths on the fly is also crucial for other techniques, such as TGA-FTIR, enabling the quantitative analysis of evolved species which has been further improved by the introduction of the pulse thermal analysis (PulseTA[®]). This method provides a quantitative calibration by relating the FTIR signals to the injected quantity of probe gas with various applications like gas adsorptions ⁽³⁾ or catalytic reactions, e.g. reduction of nitric oxides ⁽⁴⁾

References:

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