# Is it possible to get reliable and easy-to-use information from Evolving Factor Analysis?

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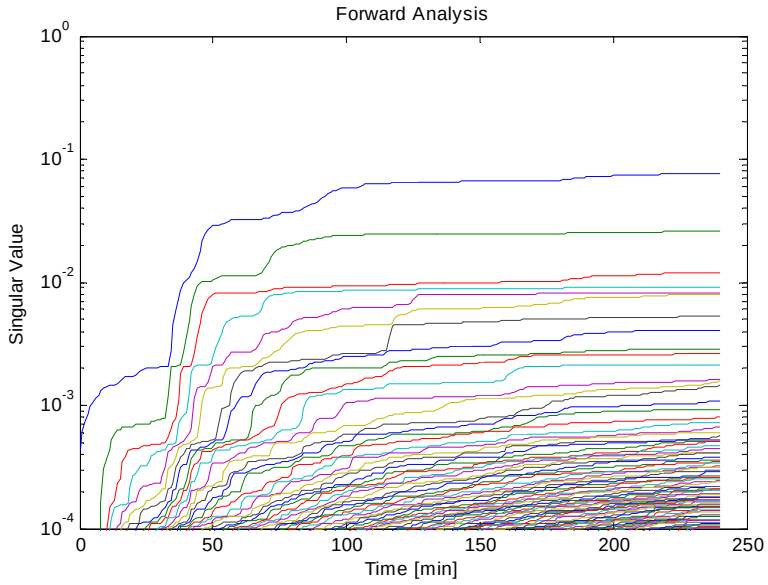
*KEYWORDS : chemometrics, EFA, reaction start/stop detection, IR, GC.*

The goal of our project (HES-SO n°11246) is to develop chemometric methods that enhance the development of chemical reactions.

Semi-batch experiments are performed at the engineering school, using a fully automated chemical reactor. Real-time analytical data, infrared (IR) spectra for instance, are synchronized with standard process variables. In parallel to the on-line measurements, the reaction is followed by conventional chemical analysis such as gas chromatography (GC).

We have chosen an aldol condensation as an example reaction. IR spectra are preprocessed (wave number region selection, filtering) and processed by Evolving Factor Analysis (EFA) to monitor the chemical reaction.

EFA is based on a sequence of principal component analysis steps and leads to a set of curves of singular values along the time axis. The time instant when a singular value leaves the bulk of random singular values is called an event. In a first step, we aim to detect the "reaction start/end point" events based on backward EFA and forward EFA respectively. The figure below illustrates forward EFA of experimental IR data of the aldol reaction.




We will present our first results about confidence intervals on the time start/end reaction points. Furthermore, we will study the influence of preprocessing and EFA parameters on these confidence intervals.