Success Story
COMET

ImPACTs
Industrial Methods for Process Analytical Chemistry - From Measurement Technologies to Information Systems
Programme: COMET – Competence Centers for Excellent Technologies
Programme line: K-Projects
COMET subproject, duration and type of project:
imPACts, 09/2014 – 08/2018, multi-firm

Chemical computers supervising the future!

Wouldn't it be nice to own the magic crystal ball providing a view on future events?
During a collaboration between the project partners FLLL, MetaDynea and RECENDT in the K-project imPACts, a tool close to that was developed: a method for chemical analytics (for instance in a melamin resin production), providing an automated maintenance strategy which is able to instantaneously alarm on upcoming drifts or errors and – on top – to autonomously correct itself, in order to immediately correct such upcoming errors.

Problem Setting

In the production of melamin resin (used in many technical applications) it is crucial to stop the polymerization reaction at the optimum moment to guarantee a product of highest quality. For that purpose, a parameter called the turbidity point has to be measured as a value corresponding to the DP (degree of polymerization). This requires time-intensive manual measurements by one or several operators, who have to draw samples from the production and perform an estimation about the current turbidity point value.

A first goal was, to reduce manual efforts while still achieving accurate turbidity point measurements. This was rather easily achieved by implementing an infrared spectroscopic measurement and corresponding chemometric models. Nevertheless, even though the received spectral data were of high quality and the generated models showed a high predictive quality on the initial on-line data, the model errors started to gradually increase after several weeks. This was also the case when the models were manually re-calibrated from time to time. The reason for such drifting situations, however, could not be clarified on a physical / chemical basis.

A solution was needed to cope with these drifts!

Solution

In a cooperation within the K-Project imPACts, researchers from FLLL developed a fully automatic calibration maintenance strategy to overcome the limitations of static chemometric models by using a combination of statistics based **drift detection**, machine learning based **model adaptation** (incl. model's knowledge expansion) and active learning.

This improved software is now able to recognize changes in the data it receives from the infrared spectrometer as early and as accurate as to detect upcoming drifts instantaneous when they occur – **before they trigger errors visible for human operators** and, above all, without any need for manual checks and reference analytics.

bmwfw
Federal Ministry of Science, Research and Economy
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The next step in the improvements is to enable the system to re-calibrate itself automatically. This so-called **model adaptation** comes in two variants:

1. Supervised adaptation based on actively selected samples: this requires some efforts from operators to gather some new reference measurements – but those efforts could be cut to about 10% compared to her/his original efforts.
2. Complete unsupervised adaptation without requiring new measurements.

Clearly, the first variant outperforms the second in terms of model accuracy, but requires a little effort from operators. So, depending on the operators' availability, one of the two variants can be chosen by the company.

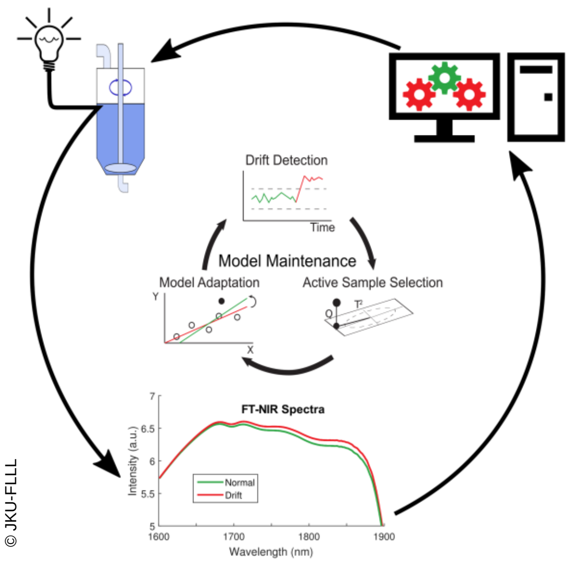

Fig. 1: Maintenance cycle and embedded methodologies, picture appears on the front cover of the July issue (Volume 1013) in *Analytica Chimica Acta*.

Results and Impact

Results on data streams from the real on-line process showed a remarkable performance of the new drift detection method: **close to 100% detection rate with no false alarms**.

Model adaptation lead to significantly lower model errors than conventional static chemometric models, finally meeting the company's requirements when using 8-10% reference measurements. With a complete cut to 0% measurements (no additional efforts for operators), the model errors were just slightly higher.

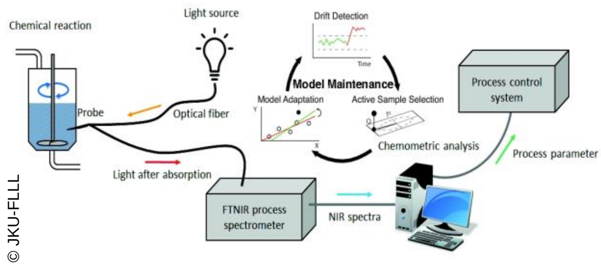

Fig. 2: This graphics shows how the maintenance cycle is embedded in the whole process control system.

The results together with the methodological concepts have been extensively described in a recently published journal article, appearing as a **featured article** in *"Analytica Chimica Acta"*, a high ranking scientific journal, with the image to the left appearing on the front cover of the special issue.

The impact for the company is very high, as it brings MetaDynea closer to a fully automatic in-line supervision system. The direct beneficiaries are the employees who don't have to bore out on tedious recurring measurements but can focus on more valuable tasks – like further optimization of the process and the product.

Contact and information

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