# Validation of PAT-based control and online data analytics in a modular plant under ATEX conditions

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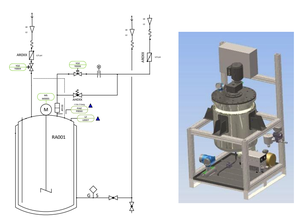
## 1. Motivation

- Novel online measurement tools and control concepts need to be validated in industrial environment (ATEX Zone 1, handling of pilot plant amounts)
- Enable a stable operation of a continuous modular production plant while achieving the desired product quality and fulfilling the safety requirements

## 2. Modular production plant

### Process Equipment Design (PED)



Documents in planning phase

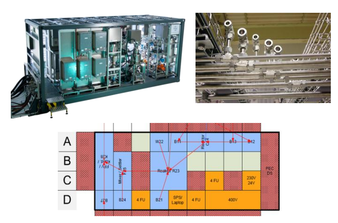
- PED contains mostly one unit operation and all supporting elements
- Design guidelines
- P&ID, Lists, 3D-CAD, cost estimation

### Process Equipment Assembly (PEA)

Physical representation of PEDs

- Follows technical and geometrical guidelines
- PEAs for unit operations and support functions

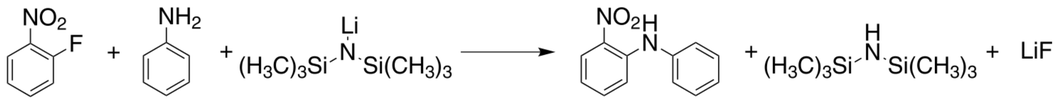
### Process Equipment Container (PEC)



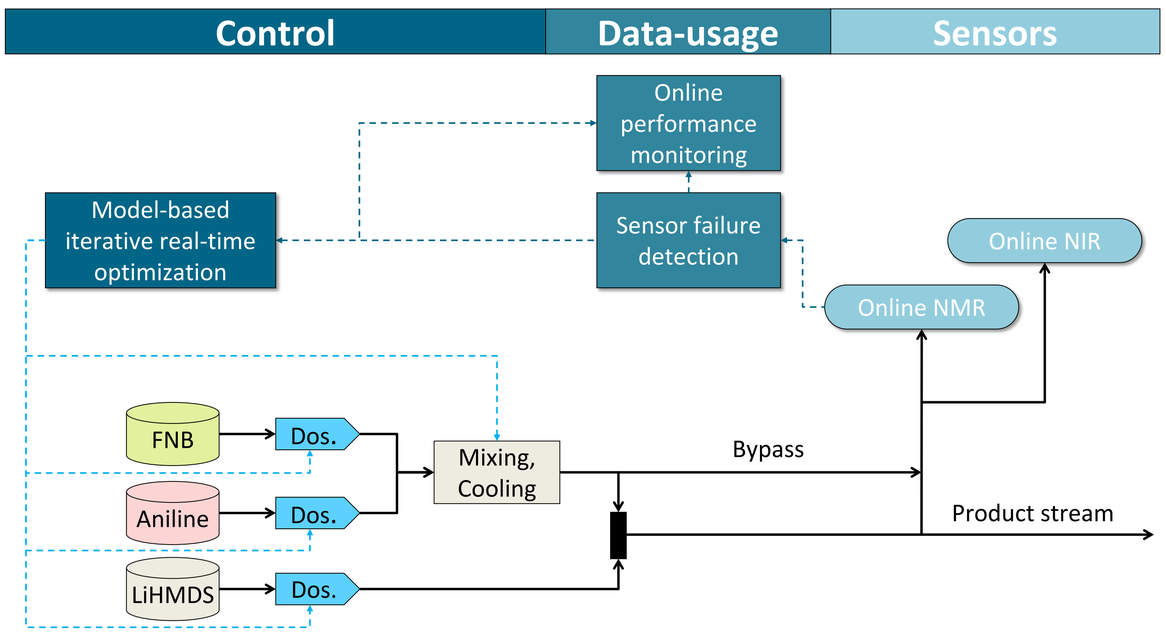
Mobile rack for plants build from PEAs

- Installation and fixation of PEAs
- Connection to energy, utilities, and process media

## 3. Case study




- Lithiation reaction with solid formation of Lithium Fluoride
- Tubular reactor without additional cooling



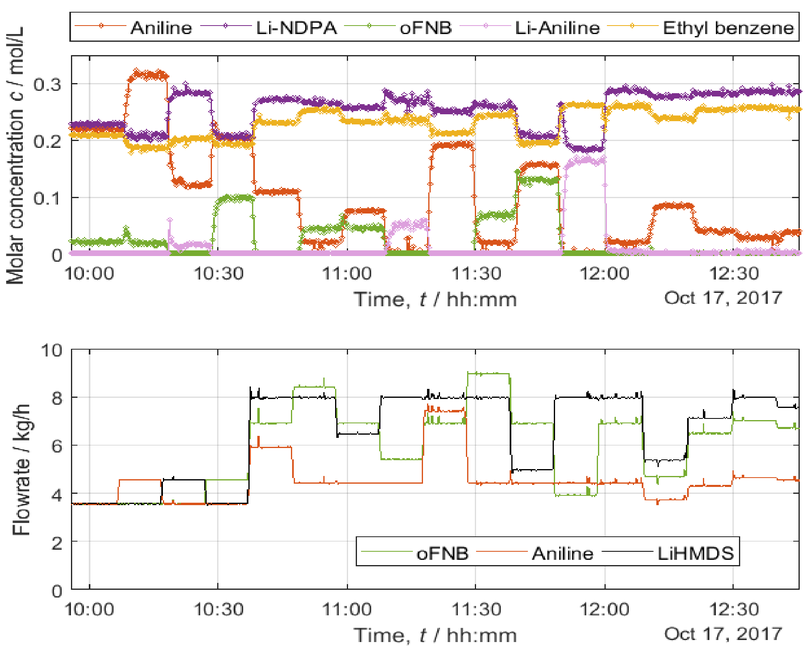

## 4. Hardware integration

Modular production plant

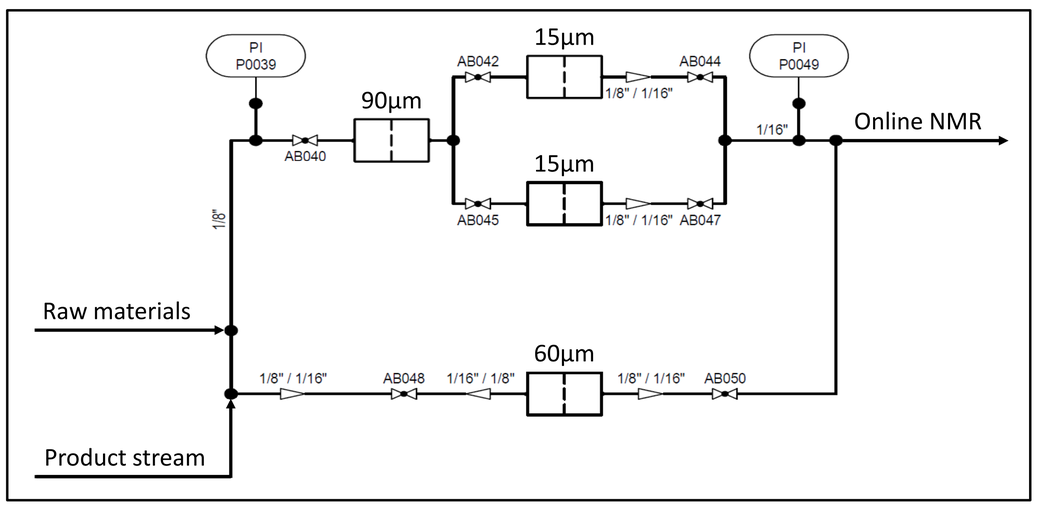
Integration of online NMR

Pressurized housing with internals

## 5. Online concentration measurements [1]



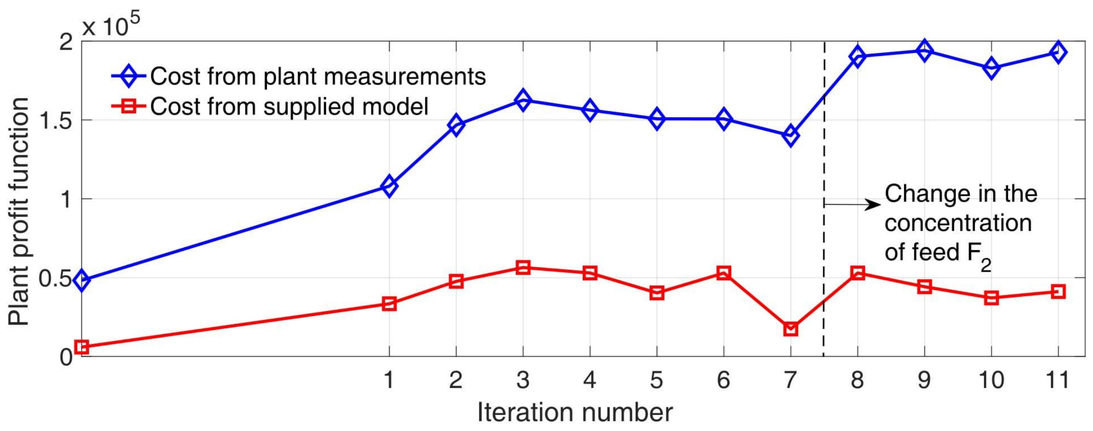

- High linearity and independent of sample matrix
- Reduced calibration effort compared to optical spectroscopy
- Short set-up times
- Fully automated data evaluation




Filter unit for solid removal

- Redundant filter elements and option to bypass during start-up phase
- Piping with capillaries (1/8”, 1/16”) and low volume filter elements to minimize residence time
- Alternating measurement of raw materials and product stream

## 6. Iterative real-time optimization [2]




- Improves the objective/profit function of the plant
- Handles plant-model mismatch
- Robust to measurement noise of NMR

## 7. Summary

- Successful implementation of online NMR and closed loop control for a hazardous lithiation reaction in ATEX Zone 1
- Benchmarking of online NMR, online NIR and offline HPLC
- Generation of further data for performance monitoring and sensor failure detection
- Demonstration that metal organic reactions can be monitored in a by-pass section without clogging with a high reliability

## References and Acknowledgements

References:
1) Simon Kern, Svetlana Guhl, Michael Maiwald, Bundesanstalt für Materialforschung und -prüfung (BAM)
2) Anwesh Reddy Gottu Mukkula, Sebastian Engell, Technische Universität Dortmund

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