

DATA FUSION STRATEGIES FOR NIR-BASED BATCH PROCESS CONTROL AND END-POINT DETECTION

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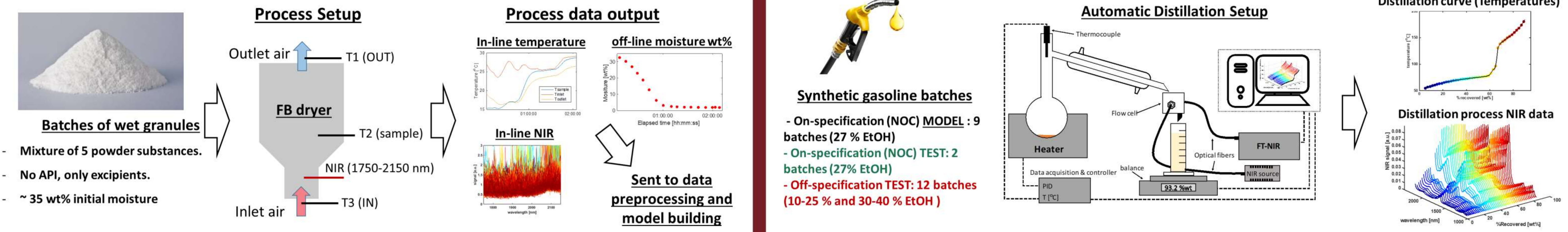
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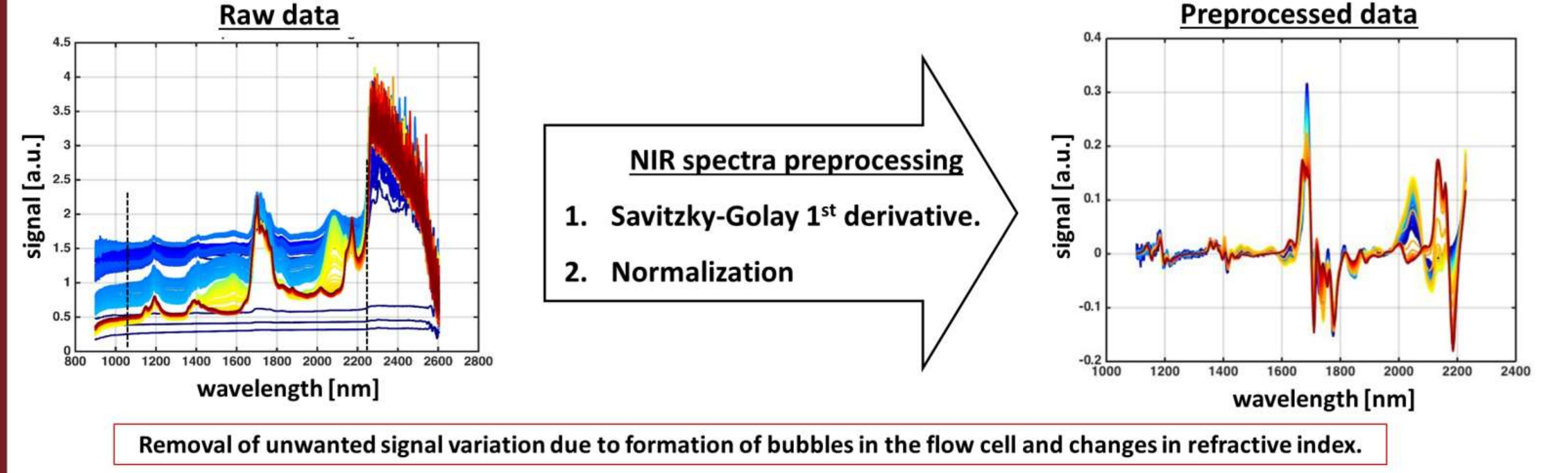
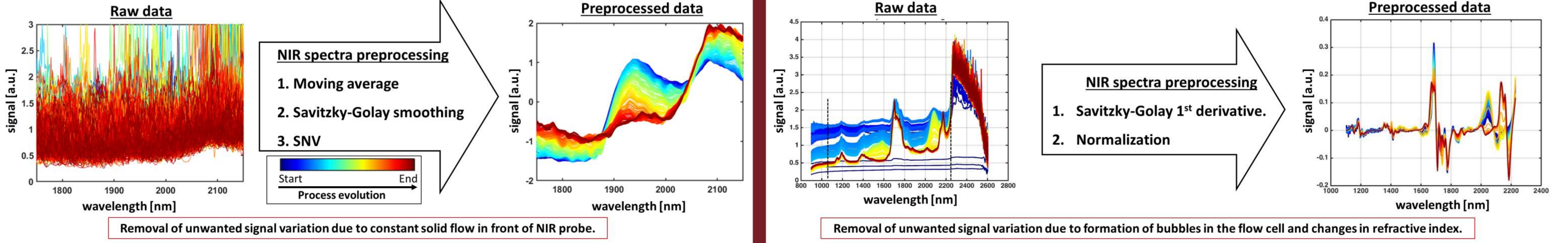
Introduction

Data fusion strategies for Multivariate Statistical Process Control (MSPC) combining diverse NIR-derived information or with other sensors were explored through real process examples. The first process is a real-time monitoring of a fluidized bed drying process of wet pharmaceutical granules. Temperature at three points of the process and NIR spectra of pharmaceutical granules were monitored in-line, while samples were collected to determine moisture content by off-line reference methods in order to build PLS models. A PCA-based MSPC model for end-point detection was built with process end-point NIR spectra. Combination of temperature readings, PLS predictions of moisture and the output of MSPC model based on the sole NIR information were used to build data fusion end-point detection MSPC. The second process is a lab-scale distillation process. Here, temperature, recovered distillation fraction and NIR spectra were acquired simultaneously. NIR data from several batches were first decomposed by multivariate curve resolution - alternating least squares (MCR-ALS). MCR-ALS compressed the original NIR data into concentration profiles of distilled fractions which were combined by mid-level data fusion with distillation temperature measurements to build on-line MSPC models for process trajectory monitoring. In all examples, NIR compressed information was separated into the part following the model (based on T^2 in PCA or concentration profiles in MCR) and out of it, i.e., residuals. Fusion is defined in a wide sense, as connecting information of different sensors or parameter-specific and general information from the same sensor.

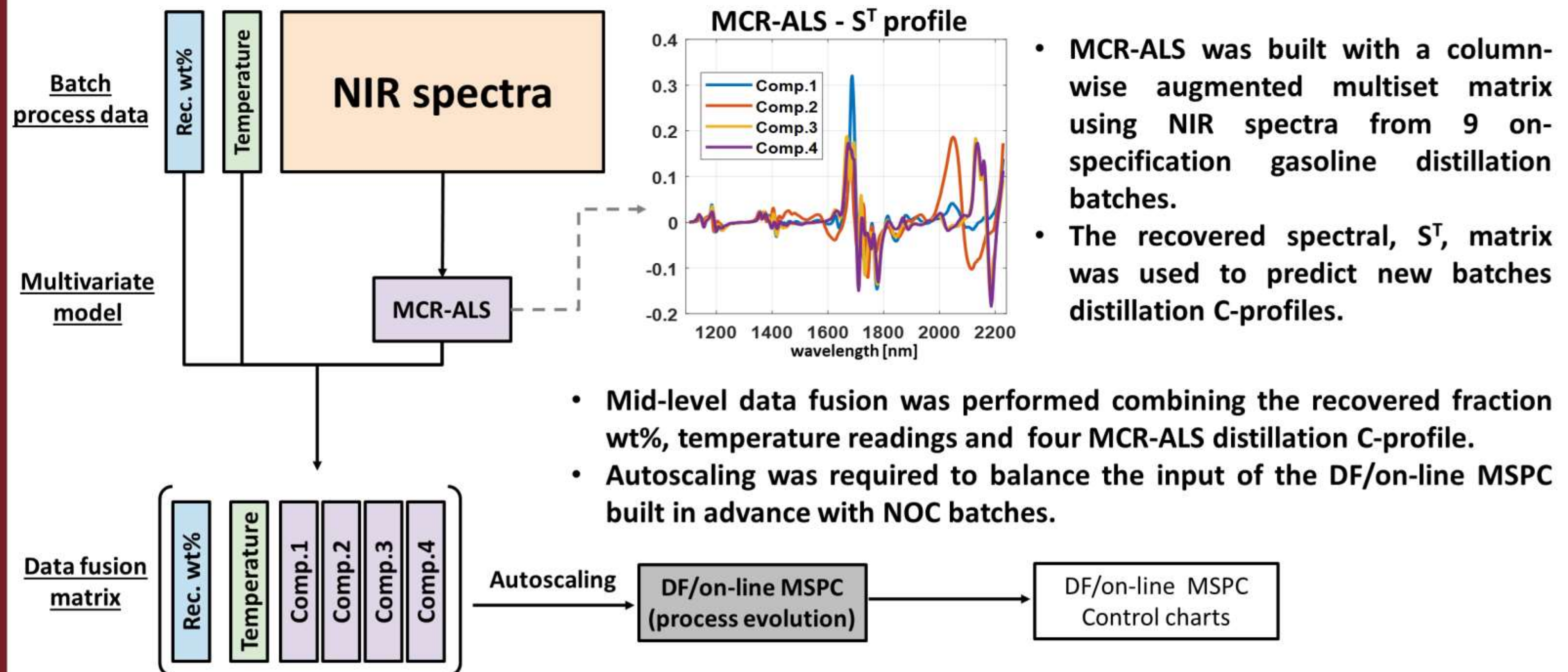
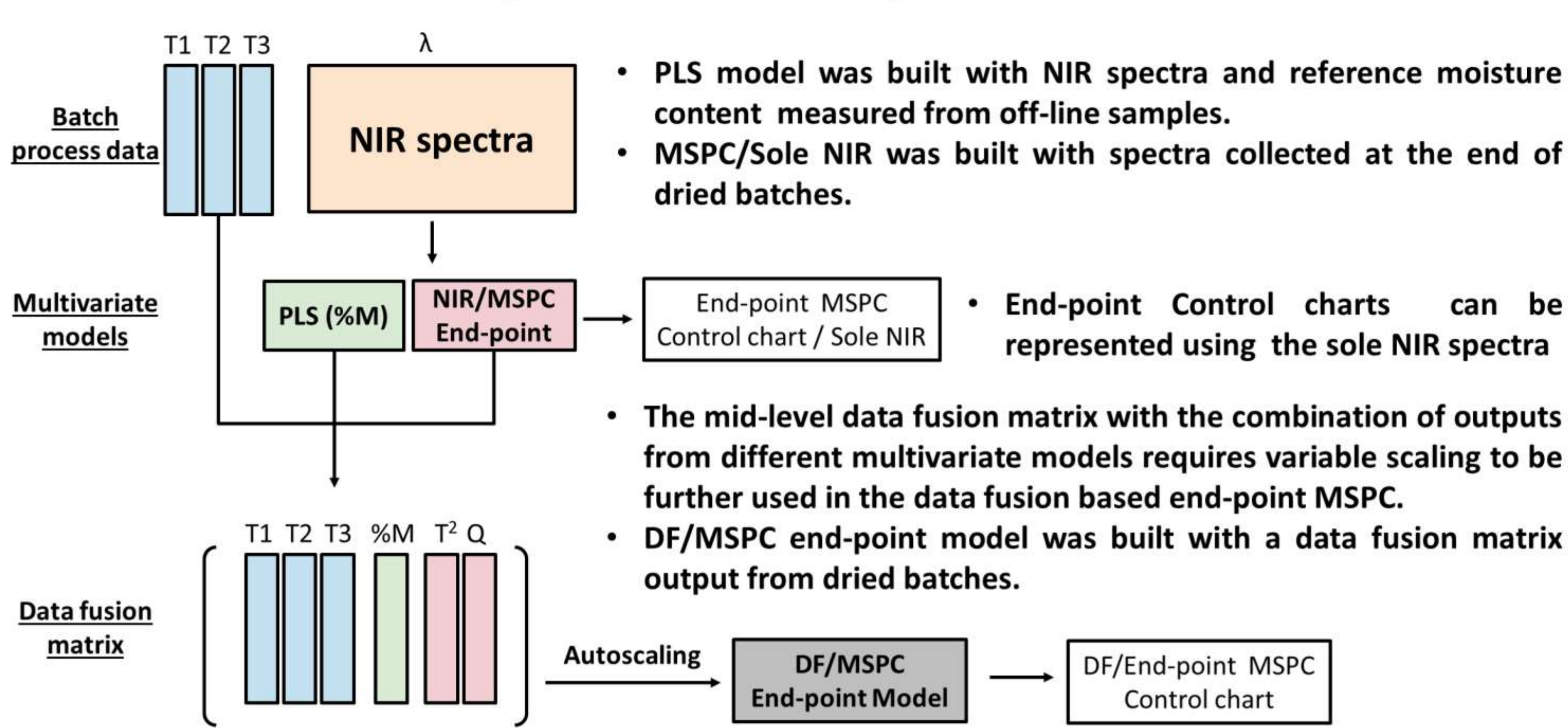
Experimental and methods



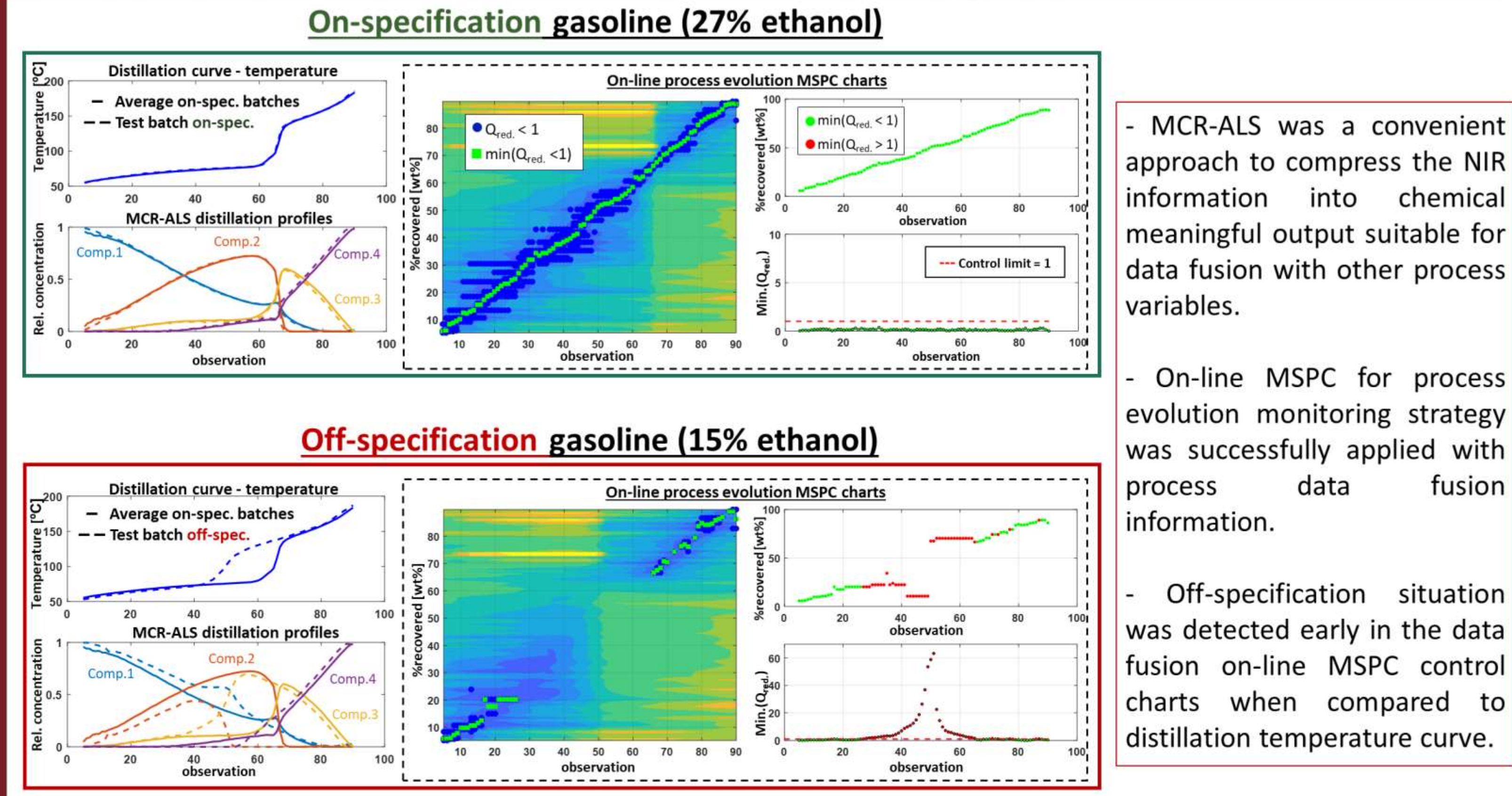
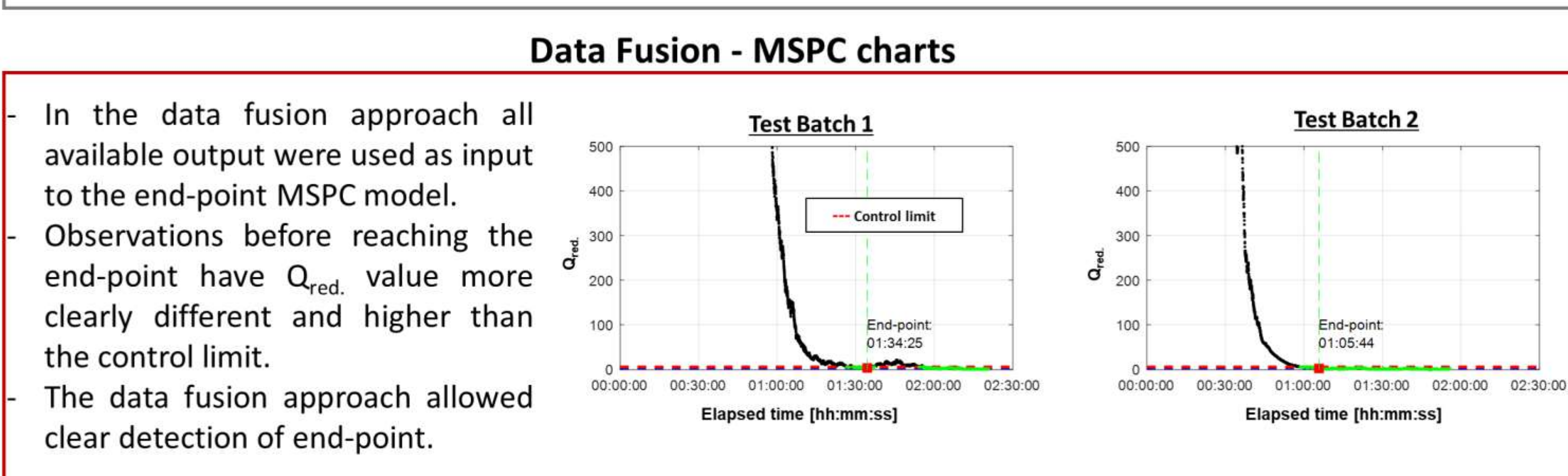
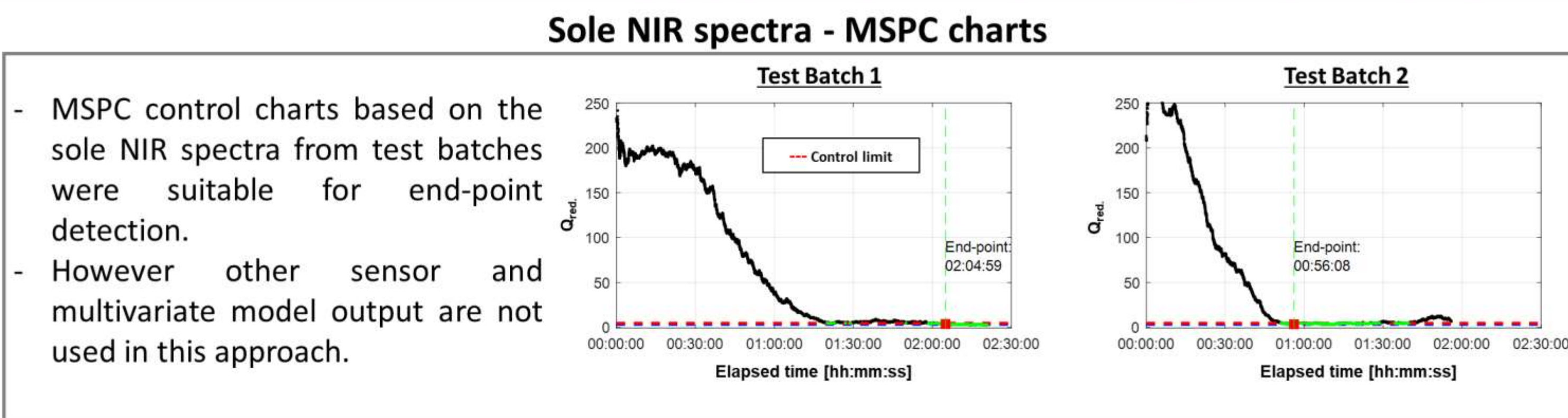
Preprocessing of NIR process data



Compression of process data and MSPC models based on mid-level data fusion



Predicted MSPC charts from test batches based on data fusion strategies



Conclusions

- MSPC models built using data fusion strategies allow providing a single answer on the performance of a process taking advantage of all the gathered information by the different sensors (or models) involved in process monitoring.
- The use of this richer information generally helps to provide clearer conclusions on off-specification situations in batch monitoring and a more accurate end-point detection that takes into account all sensor outputs and the natural correlation that should exist among them.
- The data fusion strategies presented in this work offer at the same time a general framework in terms of model building methodology and an extreme adaptability to the many diverse combinations of information that can arise due to the variability in nature and key properties to be controlled in the different processes of interest.

Acknowledgment