Scheme for Machine Learning Control of Inline Processes *Via* Real Time Spectroscopy Monitoring

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The update to Industry 4.0 is already a reality, to which machine learning and real-time monitoring are indispensable tools. In the latter's case, spectroscopy is interesting for process monitoring, with applications in sectors of biotechnology, such as food and pharmaceutical industries. Notoriously, spectroscopy monitoring is able to probe the physical state of an ongoing process in its finer details, informing about its dynamics. That information can be use to train machine learning models, which can predict the evolution of a process, as well as be used for its automation. For such a control system, three features are required: inline spectroscopy, spectroscopic data compression, and regression modeling of the process. Although studies linking pairs of those features exist in the literature, we have not found any substantial investigation joining them as a single procedure. In view of that, we have demonstrated a proof of concept for an industrial control system using machine learning and spectroscopy monitoring, as presented in Fig. 1. Our case-study process was beer mashing, monitored by Fourier-Transform Infrared (FTIR) spectroscopy, at the spectral range between 2000 and 900 cm^{-1}. For that purpose, we built an inline spectrometer and a nanobrewery at our facilities. We collected data to train a spectrum compressor (a RBF-kernel PCA model) and a reaction regressor (an Extra-Trees Random Forest model), used together for predicting the mashing dynamics. By allowing our models to control that process *via* a genetic algorithm optimizer, we observed a decrease of up to seven minutes (∼9%) in mashing time, when compared to a human-made recipe that would mash out beer wort with the same spectroscopic characteristics predicted by our models. Our findings pose meaningful contributions to current technology, which we hope to extend of various fields of industry.

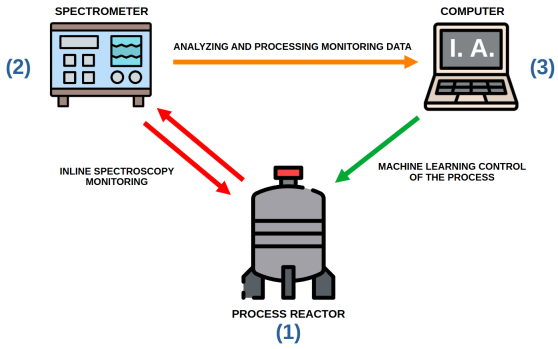

Figure 1: Process-agnostic version or our methodology for machine learning control of processes *via* spectroscopy monitoring, showing its three main components: (1) the industrial reactor where the controlled process is happening; (2) the inline spectrometer that measures the real-time state of the process; (3) the control computer on which is running the machine learning model that evaluates the monitoring data based on its evolution and commands, carrying out the process to a desired end