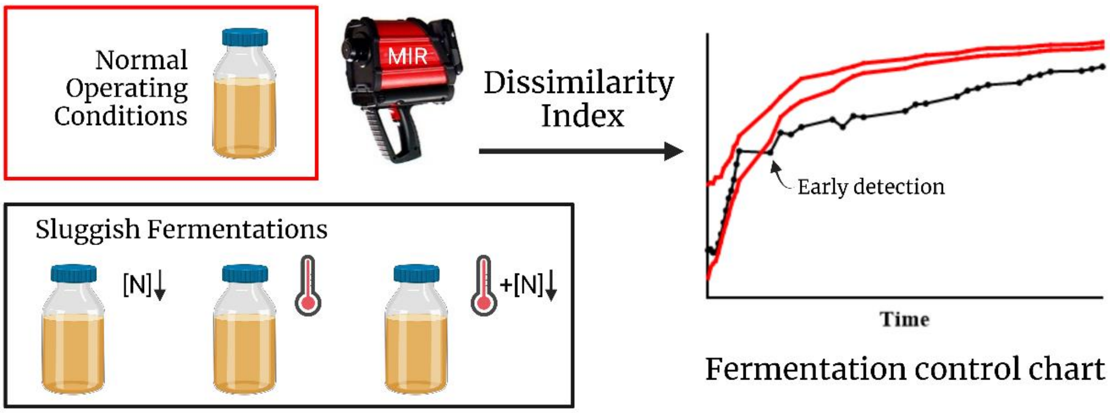
A new approach to the Dissimilarity Index as a process control tool to detect deviations in alcoholic fermentation

Daniel Schorn-García[a], Jokin Ezenarro[a], Olga Busto[a], Laura Aceña[a], Ricard Boqué[a], Montserrat Mestres[a], Barbara Giussani[b]

[a]QAQO Dpt, Universitat Rovira i Virgili, Tarragona, Spain

[b]DISAT, Università Degli Studi Dell'Insubria, Como, Italy

barbara.giussani@uninsubria.it



Food processing is highly complex due to the presence of many species, including microorganisms, which may participate in the biochemical transformations that take place. Quality control is therefore a fundamental step in all processing and production phases. Traditionally, quality control has relied on daily univariate measurements and final product characterization. However, Process Analytical Technologies (PAT), which have become popular in the pharmaceutical process, are also gaining implementation in the food and beverage sector. The concept behind PAT is to guarantee the quality throughout the entire production process [1]. Spectroscopic techniques, such as infrared, play a critical role in the implementation of PAT as they offer fast, non-destructive and in-line or on-line measurement possibilities that provide information on the molecular composition of the process [2].

Spectroscopic techniques generate multivariate data, and for this reason, Multivariate Statistical Process Control (MSPC) techniques are used to monitor and control the process. The Dissimilarity Index (DI), firstly proposed by Muncan et al. for monitoring yogurt fermentation using near-infrared spectroscopy, is based on the use of a principal component (PC) loading to describe the progress of the process [3]. Using a movingwindow approach and the first loading of the fermentation, changes in the process can be identified. The index is described as follows:

$$A_i=1-|\mathbf{p}(i)^T\mathbf{p}(0)|$$

where A_i is the dissimilarity index to detect changes between angles of the principal component loading ($\mathbf{p}(i)^T$) of the i^{th} sampling point and a reference loading $\mathbf{p}(0)$ of a preceding time.

In this research, a modified version of the DI is proposed to monitor wine alcoholic fermentation. This modified DI uses an evolving window approach and calculates de reference loading from the first hours' spectra working under Normal Operating Conditions (NOC). Then, spectra from the beginning of the fermentation to a given sampling point are considered and their first PC loading calculated and referred to the reference loading. The proposed approach was able to monitor alcoholic fermentation and, using an MSPC control chart, to detect deviations of the process. For this purpose, experiments were planned and performed by simulating temperature control problems and an initial deficit in assimilable nitrogen compounds that affect yeast metabolism. In both cases, a satisfactory detection was achieved at early stages. In addition, the effect of the deviations was studied with ANOVA–simultaneous component analysis (ASCA), showing a greater impact of the initial nitrogen concentration on the evolution of the process compared to sudden changes in temperature.

References

[1] FDA Official Document (**2004**) Guidance for Industry PAT — A Framework for Innovative Pharmaceutical Development, Manufacuring, and Quality Assurance 16.

[2] Cozzolino D (**2022**) Advantages, Opportunities, and Challenges of Vibrational Spectroscopy as Tool to Monitor Sustainable Food Systems, Food Anal Methods. **15** 1390–1396.

[3] Muncan J, Tei K, Tsenkova R (**2021**) Real-time monitoring of yogurt fermentation process by aquaphotomics near-infrared spectroscopy, *Sensors (Switzerland).* **21** 1–18.