Modelling of the production kinetics of the main fermentative aromas in winemaking fermentation

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Fermentative aromas (especially esters and higher alcohols) highly impact the organoleptic profile of young and white wines. The production of these volatile compounds depends mainly on temperature and Yeast Available Nitrogen (YAN) content in the must. Available dynamic models predict the main reaction (bioconversion of sugar into ethanol and CO2 production) but none of them considers the production kinetics of fermentative aroma compounds during the process of fermentation.
We determined the production kinetics of the main esters and higher alcohols for different values of initial YAN content and temperature, using an innovative online monitoring Gas Chromatography device. We then elaborated a dynamic model predicting the synthesis of five fermentative aromas representative of three different chemical families: two higher alcohols (isobutanol, isoamyl alcohol), one acetate ester (isoamyl acetate) and two ethyl esters (ethyl hexanoate, ethyl octanoate).
The online monitoring highlighted two successive linear phases of aroma compound production from sugar. We therefore began by modeling changes in the production yields of these compounds (aroma compound vs. sugar) depending on initial nitrogen concentration and temperature. We then integrated these yields into a previously developed model of the kinetics of sugar consumption during the fermentation process. We thus obtained a dynamic model predicting the production kinetics of volatile compounds throughout the alcoholic fermentation from initial nitrogen concentration and temperature values. The parameters of the model were identified from nine fermentations performed at temperatures between 18 and 30 ◦C and with initial YAN contents ranging from 70 to 410 mgN/L. The model was validated in six independent experiments with conditions in the same range. Predictions were accurate: the mean difference between experimental and estimated values for fermentative aroma synthesis throughout the process was below 10%, for both the fermentations used to build the model and those used for validation.
This model is the first to simulate the production kinetics of fermentative aromas and provides new insight into the synthesis of these volatile compounds. It will facilitate the development of innovative strategies for controlling the production of those aromas in winemaking, through management of the principal control factors: YAN content and temperature during the alcoholic fermentation.

Keywords:
Bioprocess monitoring, dynamic modeling, fermentation, aroma compounds, wine

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