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Selecting a best fitting mathematical model for fermentation kinetics of spontaneous wine fermentation process

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Spontaneous wine fermentation involves fermenting "grape must" using indigenous yeasts inhabiting the grapes' skin. Consistent alcohol level is crucial for producing a final product that meets quality standards in the wine industry. Therefore, this study aims to identify the most suitable mathematical model to characterize the alcohol production dynamics of indigenous yeast during spontaneous wine fermentation, with a specific focus on Sri Lanka's wine industry. The research highlights the contributions of five major indigenous yeast species: *P. kudriavzevii*, *H. guilliermondii*, *H. opuntiae*, *H. uvarum*, and *S. bacillaris*. Grape samples collected from Urumpirai, Jaffna, Sri Lanka, underwent separate fermentation processes with each yeast species, and alcohol levels were measured at regular intervals. All the experimental data sets were statistically analyzed using SPSS (version 23). The box plot analysis revealed that no outliers were detected from an initial set of 120 data points. One-way ANOVA test revealed statistically significant differences in alcohol levels across various time intervals. The kinetic parameters of the wine fermentation process were analyzed using several models, including the logistic model, the Gompertz model, the Richards model, and their respective modified versions. Among them, the modified Gompertz model became the best-fit mathematical model to describe the alcohol production patterns of each yeast species separately. The model's accuracy was evaluated using several statistical measures, such as the coefficient of determination (R^2), adjusted chi-square value, residual sum of squares (RSS), and F-value. The results demonstrated a significant variation in alcohol levels over time for each yeast species, highlighting their distinct fermentation profiles. Key parameters of the modified Gompertz model, maximum alcohol production rate ($\%v/v\ h^{-1}$), lag period (h), and upper asymptote for product formation ($\%v/v$) were estimated numerically by using the Originlab (2024) software, for each yeast species and, their alcohol production abilities were studied separately. These findings pave the way for industrial scale quality wine production using the concept of spontaneous fermentation.

Keywords: Alcohol production, Modified Gompertz model, Modified logistic model, Spontaneous wine fermentation, Yeast species