

Supplementary Materials: Temperature-Dependent Kinetic Model for Nitrogen-Limited Batch Fermentation across Yeast Species

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1. Best fits of the model to data

In this section, we provide additional information on the calibration results of the proposed model in the study. Figures S1-S10 show the best fit to fermentation time course data for batch fermentations led by five species of the *Saccharomyces* genus. The figure shows the dynamics of the yeast assimilation nitrogen, glucose and fructose uptake and the production of ethanol, carbon dioxide, glycerol, acetate, succinate, isoamyl alcohol, isobutanol and 2-phenyl ethanol in grams per liter.

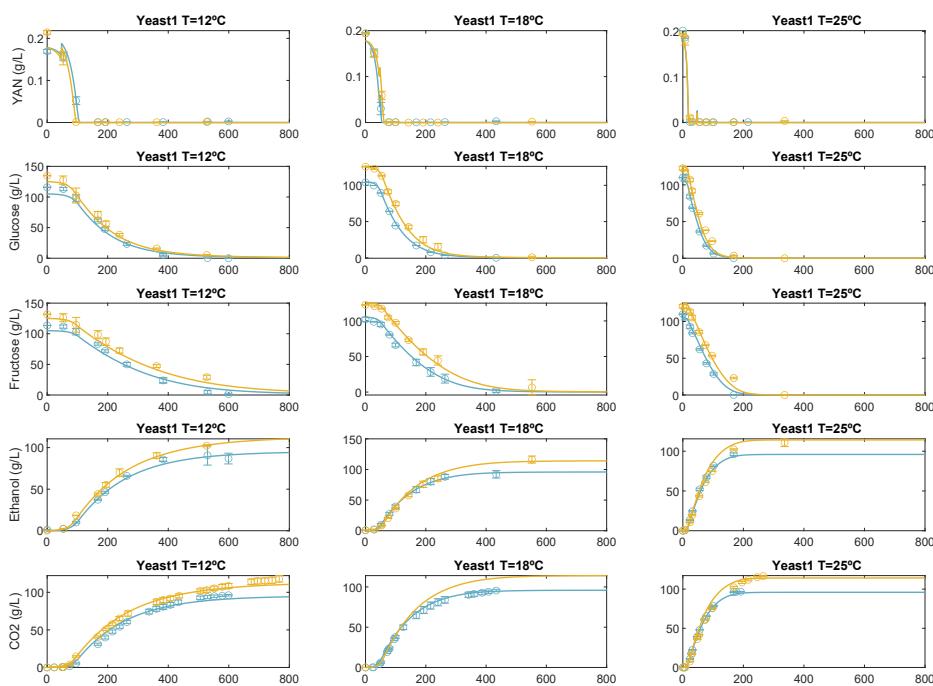


Figure S1. Best fit to the data for Yeast1: uptake of nitrogen and sugars, production of ethanol and CO₂.

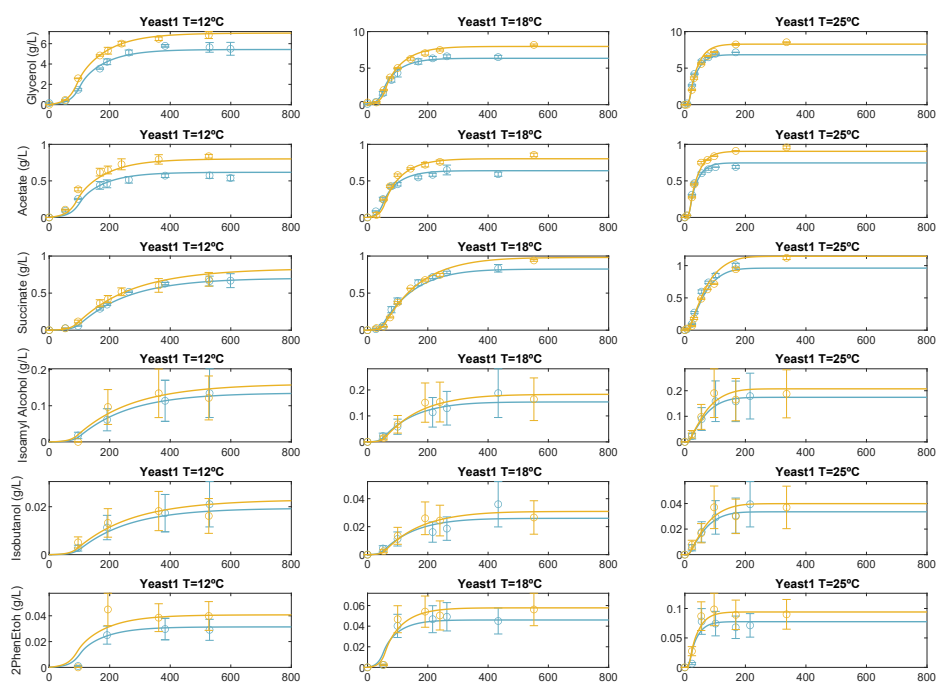


Figure S2. Best fit to the data for Yeast1: glycerol, acetate, succinate, isoamyl alcohol, isobutanol and 2-phenylethanol.

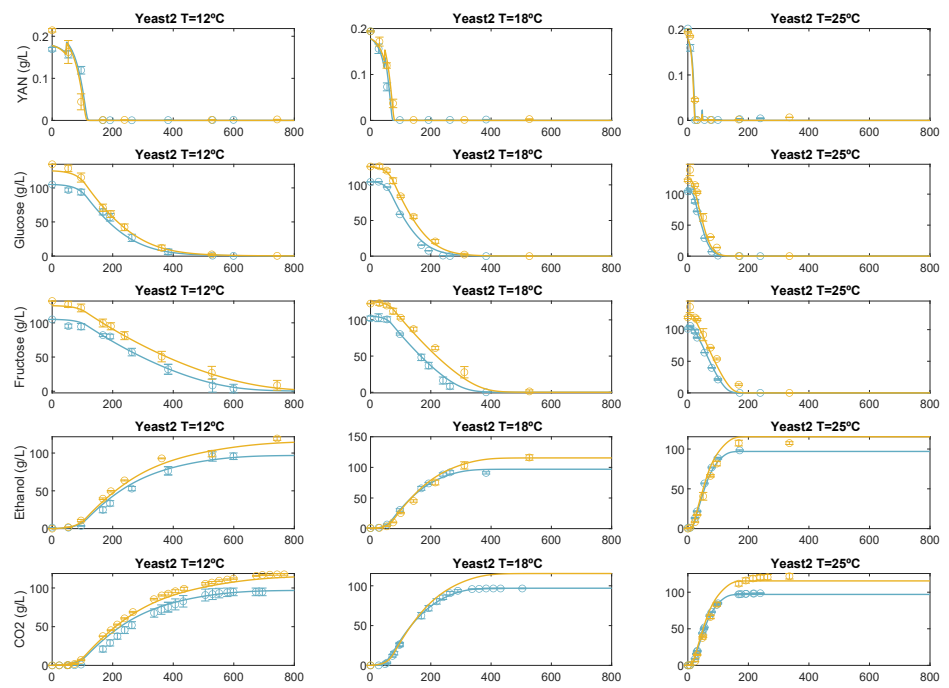


Figure S3. Best fit to the data for Yeast2: uptake of nitrogen and sugars, production of ethanol and CO₂.

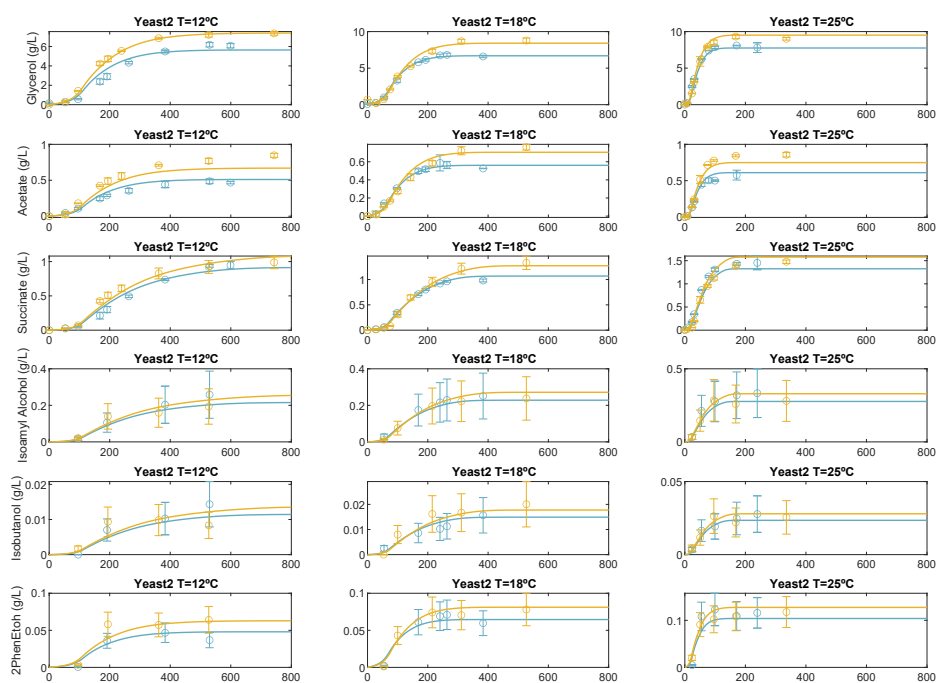


Figure S4. Best fit to the data for Yeast2: glycerol, acetate, succinate, isoamyl alcohol, isobutanol and 2-phenylethanol.

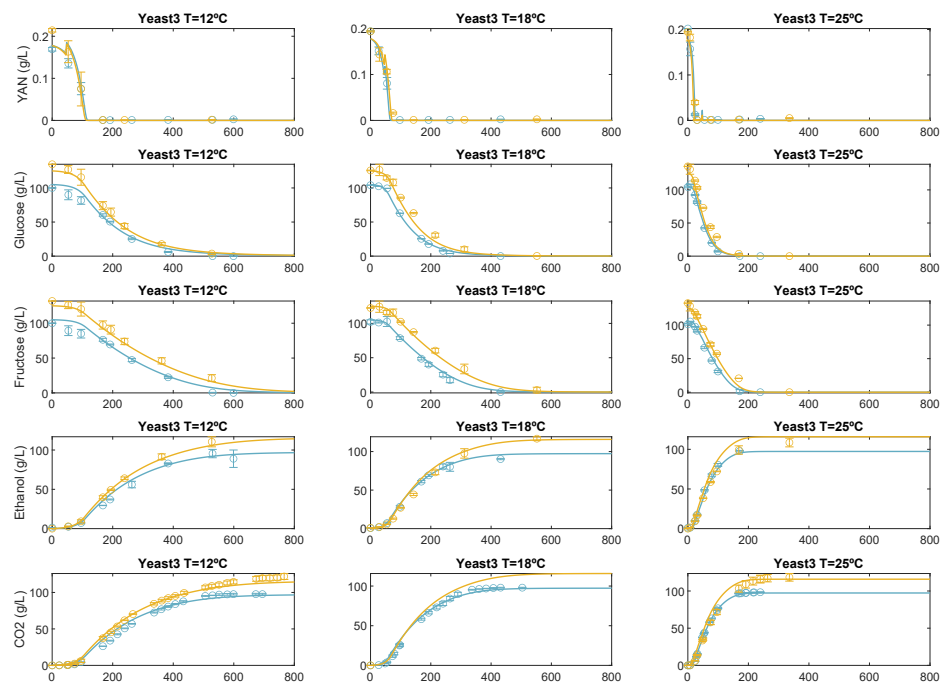


Figure S5. Best fit to the data for Yeast3: uptake of nitrogen and sugars, production of ethanol and CO₂.

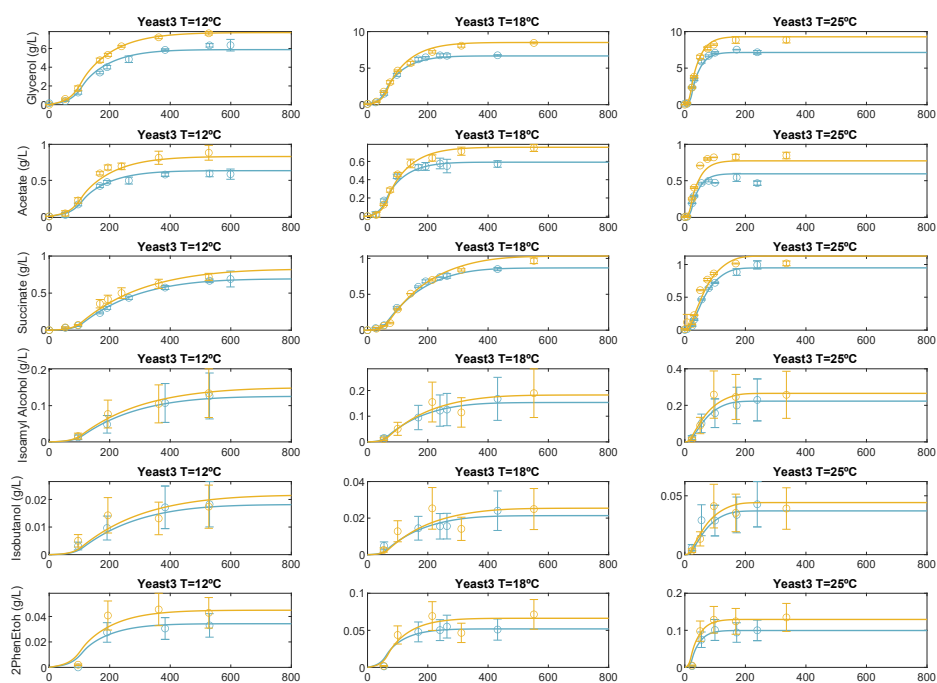


Figure S6. Best fit to the data for Yeast3: glycerol, acetate, succinate, isoamyl alcohol, isobutanol and 2-phenylethanol.

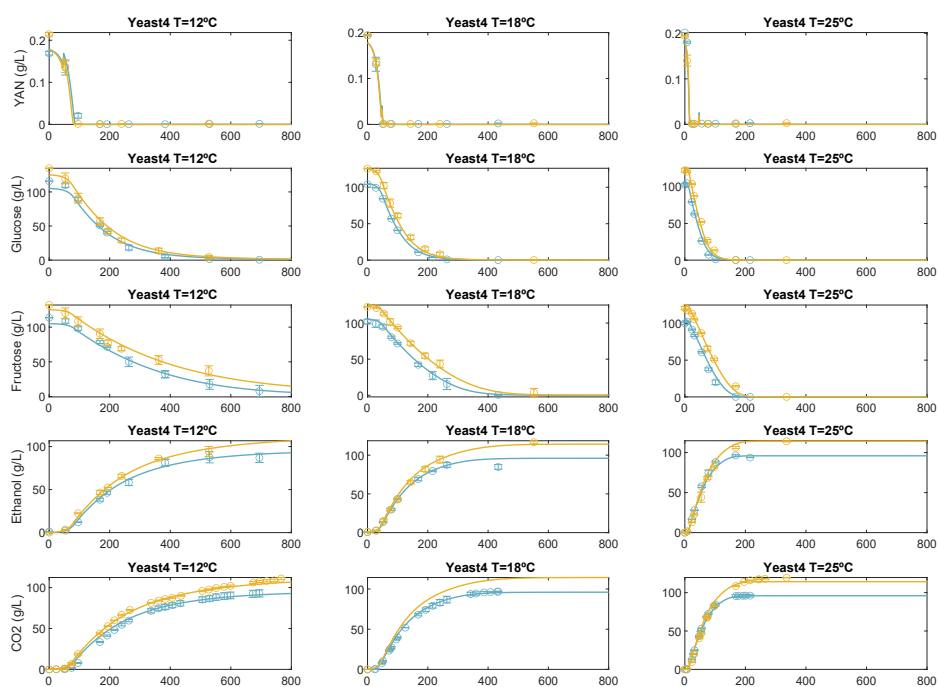


Figure S7. Best fit to the data for Yeast4: uptake of nitrogen and sugars, production of ethanol and CO₂.

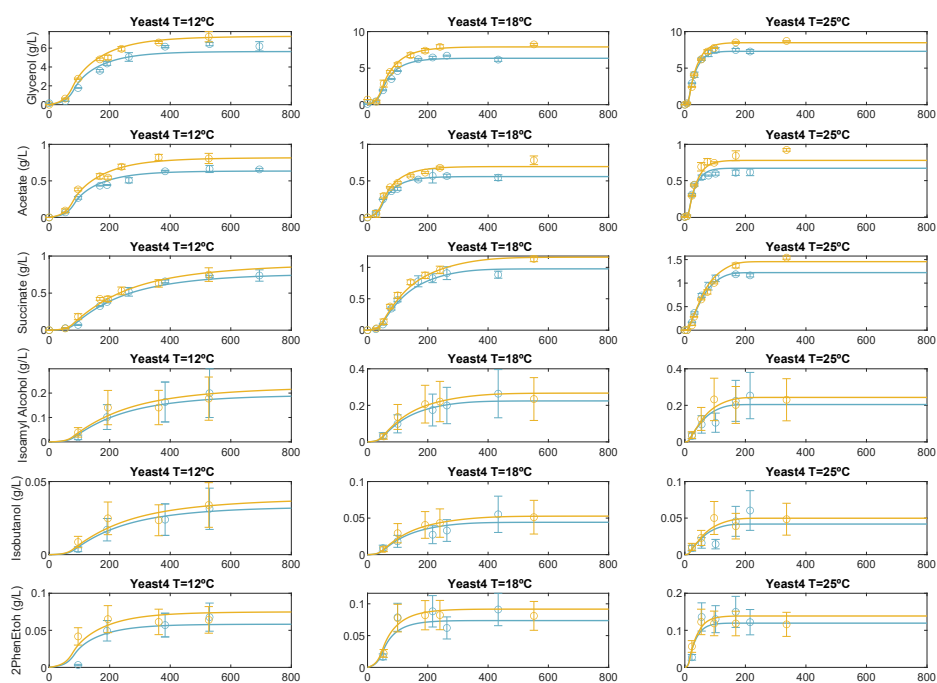


Figure S8. Best fit to the data for Yeast4: glycerol, acetate, succinate, isoamyl alcohol, isobutanol and 2-phenylethanol.

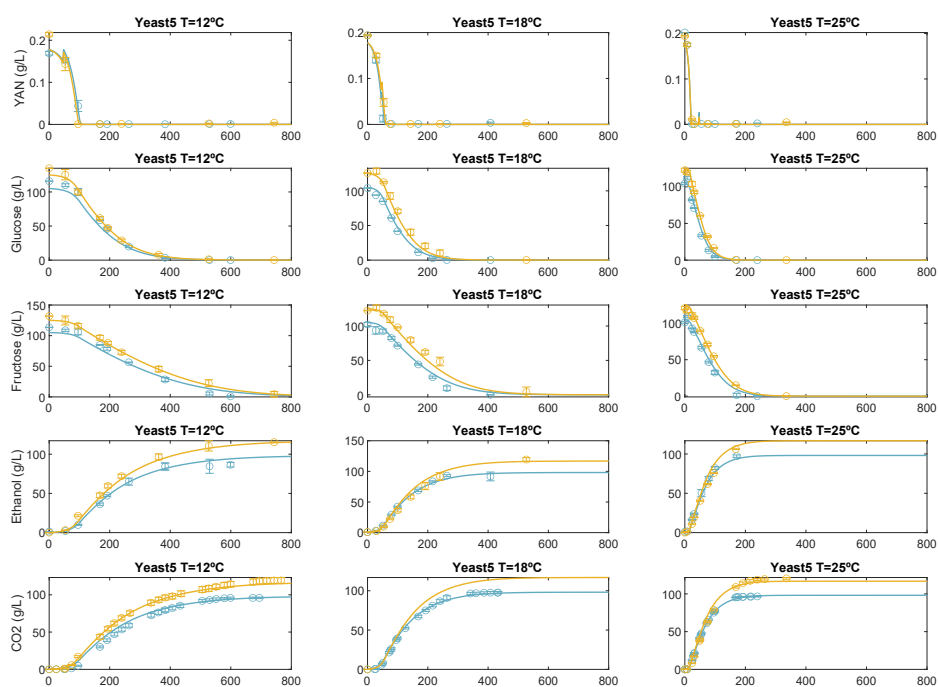


Figure S9. Best fit to the data for Yeast5: uptake of nitrogen and sugars, production of ethanol and CO₂.

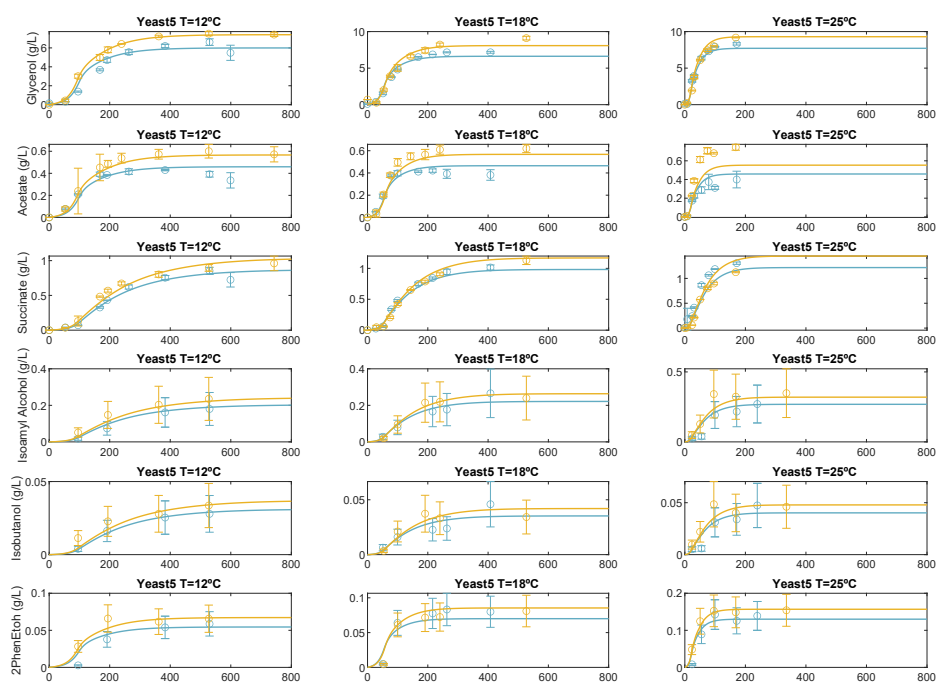


Figure S10. Best fit to the data for Yeast5: glycerol, acetate, succinate, isoamyl alcohol, isobutanol and 2-phenylethanol.

2. Strain selection in the wine fermentation illustrative example

The following supplementary figures provide a comprehensive overview of the selection process for all yeast strains analyzed in this study. We present the full set of simulation results obtained from the temperature modification analysis, covering the entire range from 12°C to 25°C in 1°C increments. These figures include all relevant state variables, such as higher alcohol concentrations, acetic acid production, ethanol yield, glycerol production, and fermentation duration. The data allow for a detailed evaluation of each strain's performance under different conditions, supporting the selection of optimal fermentation parameters. By systematically analyzing the impact of temperature on key fermentation traits, we identify strains that meet the predefined multi-objective criteria, ensuring both process efficiency and sensory quality. The results presented here serve as a complete reference, complementing the main text.

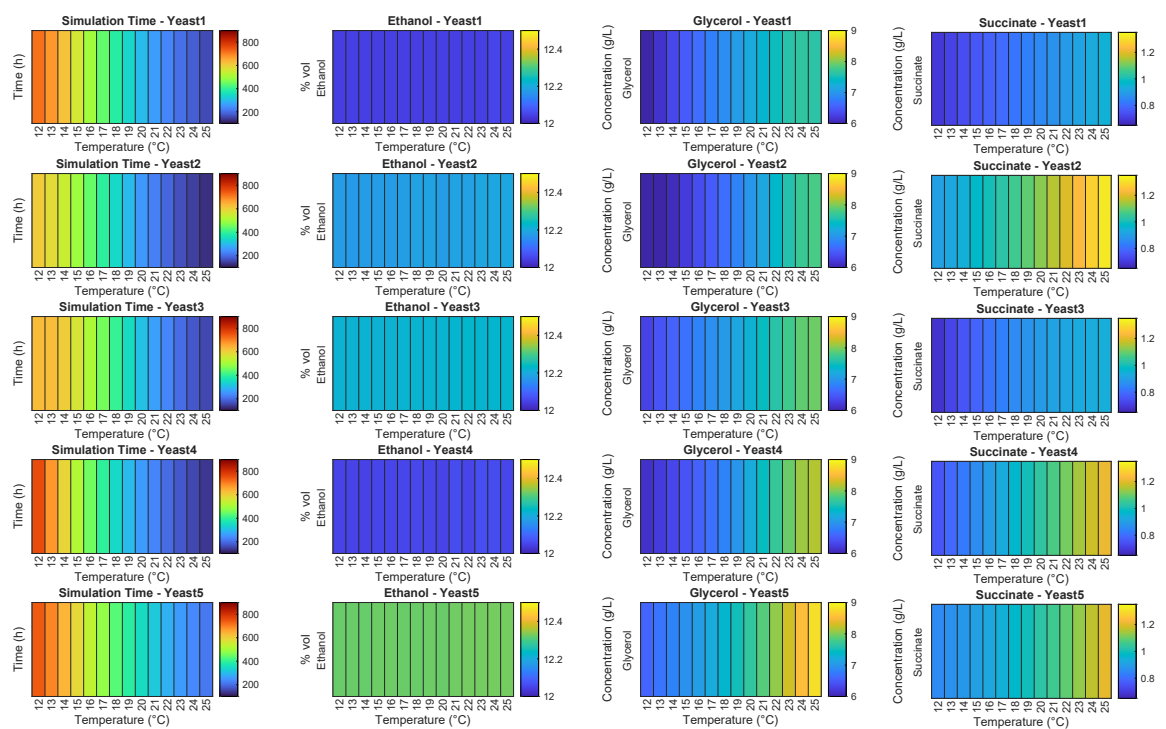


Figure S11. Simulation results obtained from the temperature modification analysis: process duration, and production of ethanol, glycerol and succinate.

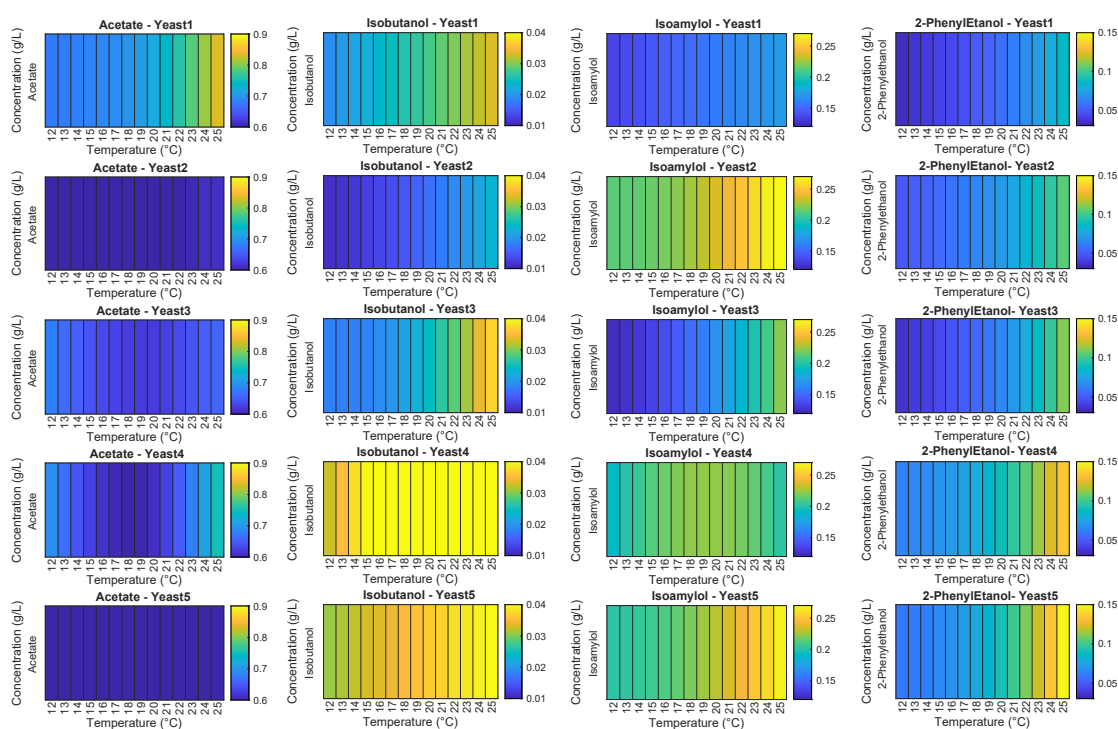


Figure S12. Simulation results obtained from the temperature modification analysis: production of acetic acid and higher alcohols.