Kinetic Model for Single-Yeast Sour Beer Fermentation

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Summary

- The implemented switch functions model changes in metabolism from aerobic to anaerobic respiration and from lactic acid production to predominantly ethanol production.
- The adaptable model proposed by Hernandez et al. was extended to describe a range of sour yeast fermentations depending on chosen independent rate parameters and initial conditions
- Acid production is associated with yeast growth and resulting pH can be calibrated via rate parameters

Modeling

Stoichiometric matrix

$$\begin{bmatrix} \frac{-M_{Glc}}{d_1 M_{Xy}} & 0 & \frac{e_1 M_E}{d_1 M_{Xy}} & \frac{f_1 M_{Gly}}{d_1 M_{Xy}} & 1 & 0 \\ \frac{-M_{Glc}}{d_2 M_{Xy}} & \frac{-b_2 M_{Ox}}{d_2 M_{Xy}} & \frac{e_2 M_E}{d_2 M_{Xy}} & 0 & 1 & 0 \\ \frac{-M_{Glc}}{d_3 M_{Xy}} & \frac{-b_3 M_{Ox}}{d_3 M_{Xy}} & 0 & 0 & 1 & 0 \\ 0 & \frac{-b_4 M_{Ox}}{d_4 M_{Xy}} & \frac{-M_E}{d_4 M_{Xy}} & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & \frac{g_1 M_{LA}}{f_2 M_{Glc}} \end{bmatrix}^T$$

Rate vector

$$\begin{bmatrix} \mu_1 \frac{G}{K_{Ga}+G} \frac{K_O}{K_O+O} \frac{K_{Ea}}{K_{Ea}+E} X_y \\ \mu_2 \lambda_r \frac{G}{K_{Go}+G} \frac{O}{K_O+O} \frac{K_{Eo}}{K_{Eo}+E} X_y \\ \mu_3 (1-\lambda_r) \frac{G}{K_{Go}+G} \frac{O}{K_O+O} \frac{K_{Eo}}{K_{Eo}+E} X_y \\ \mu_4 \frac{\delta K_{Go}}{\delta K_{Go}+G} \frac{E}{K_E+E} \frac{O}{K_O+O} \frac{K_{Eo}}{K_{Eo}+E} X_y \\ k_L a (M_O H P_O - O) \\ \mu_6 (1-\lambda_p) \frac{G}{K_{Ga}+G} \end{bmatrix}$$

Kinetic model for Lactic acid and Ethanol Production

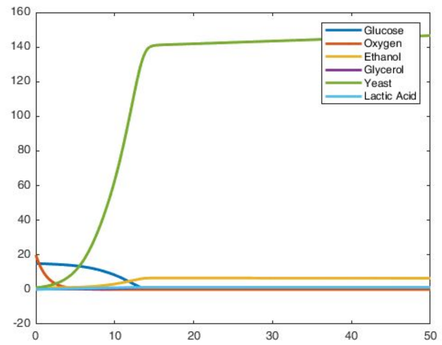
$$N^T \mathbf{R} = \frac{d\mathbf{y}}{dt}$$

The switch function rapidly inhibits lactic acid metabolism when certain specific gravity is reached

$$\lambda_p = \frac{1 + \tanh(\beta \frac{G}{S_{LA}-1})}{2}$$

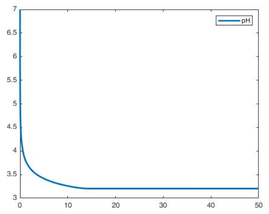
All calculations performed by ode45 in Matlab

Results

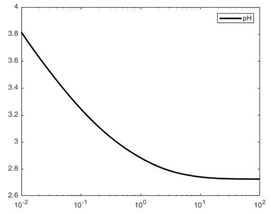


1. Overall graph of fermentation modeled

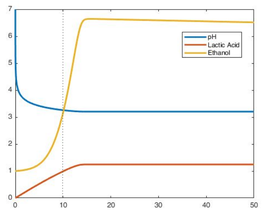
- pH is calculated at all times during the fermentation as a function of lactic acid concentration *(Fig 2)*
- The lactic acid rate constant was calibrated to yield measured pH at fermentation end through iterative modeling *(Fig 3)*
- Switch function rapidly changes fermentation metabolism which causes large changes in component concentrations *(Fig 4)*
- The lactic acid rate constant greatly affects the final composition of the fermentation *(Fig 5)*



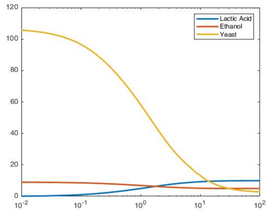
2. Change in pH vs time



3. Final pH as a function of lactic acid rate parameter



4. Concentrations of fermentation components



5. Final compositions as function of lactic acid rate parameter

Findings

- pH change occurs rapidly in the early stages of fermentation, and stabilizes as metabolism changes
- Successfully adapted experimentally verified model to sour yeast fermentation including an accurate representation of pH throughout the reaction
- Switch functions are effective in modeling key metabolic changes based upon the reaction environment
- New stoichiometric ratios and rate equations can be added to our existing model to describe more complicated fermentation reactions
- Numeric integration can be used to combine an interdependent system of rate equations to describe the concentrations of reactants throughout a reaction

Next Steps

- Increase flexibility and accuracy of model by expanding range of inputs to the model
- Account for more complex worts by including maltose and maltotriose in rate expressions
- Apply and calibrate model to lab fermentation
- Use model to predict fermentation products

References

1. González-Hernández, Y.; Michiels, E.; Perré, P. A Comprehensive Mechanistic Yeast Model Able to Switch Metabolism According to Growth Conditions. Fermentation 2022, 8, 710. https://doi.org/10.3390/fermentation8120710
2. J. Gee DA, Ramirez WF. Optimal temperature control for batch beer fermentation. Biotechnol Bioeng. 1988 Feb 20;31(3):224-34. doi: 10.1002/bit.260310308. PMID: 18584597.