

# Model-based dynamic optimization of the microbial production of lignocellulosic bioethanol in fed-batch bioreactors

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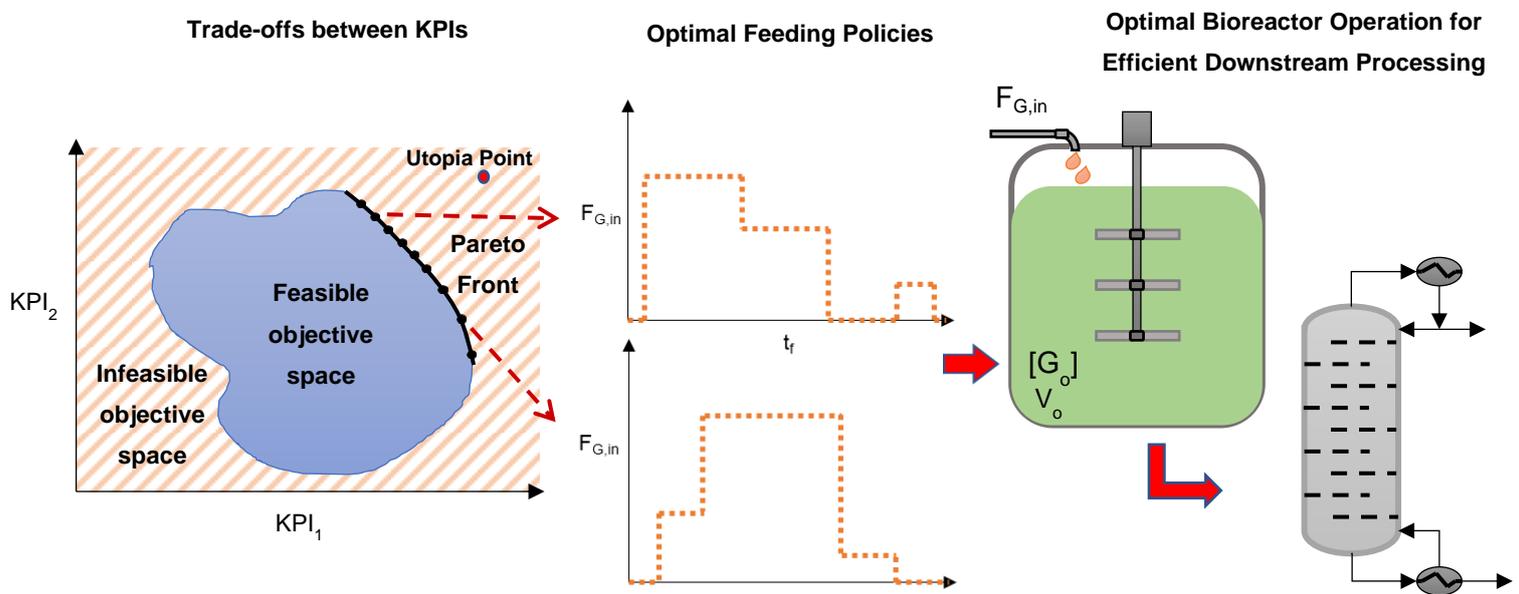
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## 1. Introduction

The synergistic action of multiple inter-disciplinary sectors (engineering, business, law) is a prerequisite to harness the full potential of lignocellulosic biomass processing technologies. In the case of the biofuel production, lignocellulosic bioethanol, also known as second-generation bioethanol, is considered a sustainable alternative to fossil-based and first-generation fuels. However, from an engineering standpoint, the establishment of second-generation bioethanol as a viable competitor to its unrenowable counterparts requires appreciable cost reductions. The optimal operation of the fermentation bioreactor constitutes a primary driver to enhance overall process performance and competitiveness. This study investigates the model-based dynamic optimization of the fermentation process by simultaneously maximizing key performance indicators (KPIs). The economic dimension of the optimal operating policies is marked out to identify promising operational designs, accounting for implications at the downstream process stage, as a means of improving second-generation bioethanol plant economics.

## 2. Methods

Fermentation is simulated by a mechanistic model validated against lab-scale experimental data [1]. Process performance is assessed through three KPIs, namely productivity, yield and final bioethanol concentration. The proposed optimal operating strategies are produced by handling the initial liquid culture volume ( $V_0$ ), the initial glucose concentration ( $[G_0]$ ), the glucose feeding rate ( $F_{G, in}$ ) and the fermentation time ( $t_f$ ). The conflicting KPIs are maximized individually, as well as simultaneously through a multi-objective optimization approach, where the trade-off solutions are obtained via the modified Tchebycheff method. The economic benefit of the trade-off solutions is evaluated via a sophisticated index incorporating the hydrolysate glucose production cost. Finally, the robustness of the economic index's value in the presence of uncertainties associated with model parameters is assessed via rigorous Monte-Carlo simulations. These uncertainties can be thought of as irregularities in cellular metabolism as the bioreactor scale increases from lab- to industrial-scale.



**Figure 1:** Multi-objective optimization approach

### 3. Results and Discussion

It is demonstrated that the attainment of high values in productivity with substantial compromises in yield and final bioethanol concentration is a condition that should be the focal point of bioreactor operating design in order to enhance economic feasibility in lignocellulosic bioethanol plants. Furthermore, the optimal policy yielding the highest economic benefit corresponds to a fermentation performance ( $3.32 \text{ g L}^{-1} \text{ h}^{-1}$ ,  $0.399 \text{ g g}^{-1}$ ,  $106.0 \text{ g L}^{-1}$ ), which is competitive to that reported for first-generation bioethanol. This constitutes a step forward towards the commercial establishment of lignocellulosic bioethanol plants. Nonetheless, perturbations in cellular metabolism appear to have an appreciable impact on bioreactor performance even under the implementation of optimal operating schemes.

### 4. Conclusions

The transition to continuously operating bioreactors could lead to further improvement in productivities; however for this endeavour to be successful, deeper insight into yeast metabolism and population heterogeneity is required to devise control strategies that can efficiently guide the culture toward desirable steady states.

### References

- [1] A. Karapatsia, G. Penloglou, C. Chatzidoukas, and C. Kiparissides, "Fed-batch *Saccharomyces cerevisiae* fermentation of hydrolysate sugars: A dynamic model-based approach for high yield ethanol production," *Biomass and Bioenergy*, vol. 90, pp. 32–41, 2016.