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Energy-optimal control of temperature for wine fermentation based on a novel model including the yeast dying phase ⋆

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Abstract: We study energy-optimal control of the cooling process during wine fermentation. The process of wine fermentation is described by a novel model (Borzì et al. (2014)) including a death phase for yeast and the influence of oxygen on the process. The parameters determining the fermentation dynamics are estimated from measurements and the optimal cooling profile is computed. The numerical results regarding the development of the substrates and the product as well as the control profiles for a common fermentation temperature profile and the optimal temperature profile are compared. It turns out that significant improvement can be achieved by using the optimal calculated temperature profile.

Keywords: control applications, temperature control, fermentation processes, dynamic models, system models, ordinary differential equations, parameter and state estimation

1. INTRODUCTION

The main objective of industrial enterprises consists in increasing their profit. This means that the profit of any product should be increased. One way to the solution of this profit-driven objective is to reduce production costs but maintain or improve the quality of this product at the same time. Therefore, the application of mathematical simulation and optimization methods establishes more and more in industry. In the context of wine fermentation, this is the main objective of the project RŒNOBIO.
There is a high savings potential for energy consumption in the process of making wine. In 2009 the energy requirements caused 0.08% of the global greenhouse gas emissions or in other words about 2 kg/0.75l bottle (Smyth et al. (2011)). Exemplary in California the annual energy consumption in wine industry is located at 400 GWh, the second highest in food industry (Galitzky et al. (2005)). Thereby the control of the fermentation temperature has a high impact. (Freund (2009); Bystricky (2009); Freund et al. (2008)). That is why it is of significant importance to minimize the energy needed for cooling during wine fermentation.
In Borzì et al. (2014), a novel model for wine fermentation including the yeast dying phase has already been presented. This model reflects the behavior of yeast cells that is observed in reality apart from the lag phase taking place at the beginning of fermentation. The yeast growth phases are illustrated in Dittrich and Gromann (2011). Furthermore, it takes oxygen into account which is an important factor for yeast activity.
In addition to this, for solving an energy-optimal control problem controlling the fermentation temperature, the temperature development has to be included in the model. The conversion of sugar into alcohol is an exothermic reaction which means that heat is produced. This heat has to be dissipated as temperature plays a crucial role for yeast. If the fermentation temperature is too high, yeast cells die. However, in the phase where oxygen is present, even more heat is produced.
In this paper, the parameters included in this new model describing the wine fermentation process are identified from measurements. Then, by making use of these estimates an optimal control problem (OCP) for minimizing the cooling energy, needed during the fermentation process by controlling the fermentation temperature, is studied.
In section 2, the model representing the wine fermentation process is introduced, and then the considered optimal control problem is mentioned in section 3. Subsequently, the methods for estimating the involved parameters and for the solution of the introduced energy-optimal control problem are presented in Section 4. Afterwards, results regarding the parameter estimation (PE) using multiple experiments and a comparison of results for a common temperature profile and an optimal temperature profile are shown in Section 5. Conclusions are presented in Section 6.

2. PROCESS MODEL DESCRIPTION

First, we recall the model introduced in Borzì et al. (2014) in (1). It describes the wine fermentation process as it can be observed in real experiments.
In this model, the growth of yeast concentration is dependent on the consumption of the nitrogen, sugar and oxygen concentration. Sugar is converted into alcohol but inhibited by it as well.
Here, the sugar concentration is split up into two parts, the amount of sugar which is converted into ethanol and the amount of sugar needed as a nutrient for the yeast. Besides this, the presence of oxygen is considered in this

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model because it plays a crucial role for yeast activity, especially in the case of using a Saccharomyces cerivisae yeast strain.

$$\begin{cases} \dfrac{\partial X}{\partial t} = \mu_{max}(T)\dfrac{N}{K_N+N}\dfrac{S}{K_{S_1}+S}\dfrac{O_2}{K_O+O_2}X \\ \quad -\Phi(E)X \\ \dfrac{\partial N}{\partial t} = -k_1\mu_{max}(T)\dfrac{N}{K_N+N}\dfrac{S}{K_{S_1}+S}\dfrac{O_2}{K_O+O_2}X \\ \dfrac{\partial E}{\partial t} = \beta_{max}(T)\dfrac{S}{K_{S_2}+S}\dfrac{K_E(T)}{K_E(T)+E}X \\ \dfrac{\partial S}{\partial t} = -k_2\dfrac{\partial E}{\partial t} \\ \quad -k_3\mu_{max}(T)\dfrac{N}{K_N+N}\dfrac{S}{K_{S_1}+S}\dfrac{O_2}{K_O+O_2}X \\ \dfrac{\partial O_2}{\partial t} = -k_4\mu_{max}(T)\dfrac{N}{K_N+N}\dfrac{S}{K_{S_1}+S}\dfrac{O_2}{K_O+O_2}X \end{cases} \tag{1}$$

The death of cells, included in the differential equation for yeast, is modeled by the following nonlinear term

$$\Phi(E) = \left(0.5 + \frac{1}{\pi}\arctan(k_{d_1}(E-tol))\right)k_{d_2}(E-tol)^2, \tag{2}$$

where tol represents the tolerated ethanol concentration. Besides this, k_{d_1} and k_{d_2} are parameters associated to the death of yeast cells due to ethanol exceeding the tolerance tol. This death term assures that the lag and death phase of yeast cells take place. The development of yeast cells in these phases depends on the concentration of ethanol. Alcohol inhibits the yeast such that if its concentration is below a tolerance tol the number of yeast cells stays stationary, and if it is greater than tol, the yeast cells die.

X represents the yeast concentration, N the nitrogen concentration, E the ethanol concentration, S the sugar concentration, O_2 the oxygen concentration and T the time-dependent temperature.

This model makes use of Michaëlis-Menten kinetics. Here, the specific growth rates $\mu_{max}(T)$ and $\beta_{max}(T)$ are dependent on temperature T. Furthermore, K_N and K_O are the Michaëlis-Menten half-saturation constant associated to Nitrogen and Oxygen. Besides this, $K_E(T)$ shows the ethanol inhibition dependent on temperature. The parameters k_1 and k_4 are the yield coefficients associated to nitrogen and oxygen respectively.

In this model, two saturation constants associated to sugar, namely K_{S_1} and K_{S_2}, are needed. Thereby K_{S_1} represents the saturation constant associated to the part of sugar used as a nutrient for the yeast and K_{S_2} is the saturation constant associated to the part of sugar needed for the metabolization into alcohol. Moreover, also two yield coefficients associated to sugar are needed. On the one hand, there is k_2 which represents the yield coefficient associated to the part of sugar that is converted into alcohol and on the other hand, there is k_3 which stands for the yield coefficient related to the part of sugar which is used as a nutrient for the yeast.

3. OPTIMAL CONTROL PROBLEM

In industry, the main goal is to increase the profit of a product. This means that the focus mostly lies on reducing the production costs without sacrificing the quality of the product. Thus, our objective in the OCP, formulated below, is the minimization of the energy needed for cooling by controlling the fermentation temperature together with constraints on the maximum temperature and the ethanol output, expressed by a boundary condition (equation (17)).

The control variable u is a temperature flux over time.

$$\min J(u) := \int_0^{t_f} |T_{ext} - u(t)|dt$$

$$\text{s.t.} \quad \begin{cases} \quad \text{Model (1)} \\ \dfrac{\partial T}{\partial t} = \alpha_1\dfrac{\partial E}{\partial t} - \alpha_2\dfrac{\partial O_2}{\partial t} - \alpha_3(T-u) \end{cases} \tag{3}$$

with adequate initial values, box constraints and as already mentioned a boundary condition regarding the final ethanol concentration.

Furthermore, the development of temperature has to be observed. Thereby it is assumed that with the accumulation of ethanol, the temperature inside the fermentation tank rises and with the presence of oxygen even with a higher impact. These components are represented by the differential equation for temperature. So, α_1 represents how much heat is produced by the conversion of sugar into alcohol. Moreover, α_2 expresses the measure of how the presence of oxygen intensifies this accumulation of heat. α_3 can be interpreted as a diffusion coefficient which is the smaller the greater the wine tank in relation to the cooling element is. Thereby T is the current temperature in the fermentation tank and u the temperature of the cooling fluid flowing through the cooling element which is the control in this OCP.

The objective $J(u)$ consists in minimizing the energy needed for cooling during fermentation. This means that the absolute difference between the exterior temperature (the temperature outside of the tank) and the temperature control integrated over time is calculated.

4. COMPUTATIONAL METHODS

In this section the techniques for estimating the parameters and solving the OCP presented in section 3 are explained.

A parameter estimation problem (PEP) is a subclass of an optimal control problem and there are several different ways of solving OCPs as described in Binder et al. (2001).

In our case, a direct multiple shooting approach (Plitt (1981); Bock and Plitt (1984); Bock (1987)) was chosen for the discretization of the PEP (4) and of the OCP (3), a backward differentiation formula method (BDF method, as in Hairer (2010)) for the numerical integration of the system of ordinary differential equations and a sequential quadratic programming method (SQP method, as in Nocedal and Wright (2006)) for the solution of the resulting constrained nonlinear optimization problem.

These methods were implemented using the ACADO toolkit - a toolkit for Automatic Control and Dynamic Optimization developed by Moritz Diehl et al. (Ariens et al. (2010–2011);