Less cooling energy in wine fermentation - a case study in mathematical modeling, simulation and optimization

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Abstract

In this paper, we study model predictive control (MPC) of the cooling process during wine fermentation. A strategy to solve nonlinear control problems with changing model parameters, unknown disturbance factors and changes in the states is presented. The parameters and states determining the fermentation dynamics are regularly estimated from measurements and the optimal cooling profile is computed and if necessary adjusted. The process of wine fermentation is described by a slightly modified version of the novel model including a death phase for yeast and the influence of oxygen on the process published in Schenk et al. (2014). The numerical results regarding the control inputs and the development of the substrates and the product for an industrial controller and for this MPC controller are compared. It arises that the usage of this MPC cooling strategy results in considerable savings for the energy consumption in the process of wine fermentation.

Keywords:

control applications, model predictive control, temperature control, fermentation processes, parameter and state estimation

1. Introduction

For industrial companies the main objective consists in making profit. One way to increase the profit of a company is to increase the profit of any product by reducing its production costs but maintaining its quality at the same time. Therefore, the application of mathematical modeling, simulation and optimization techniques establishes more and more in

industry. In the context of fermentation processes, this is the main objective of the project RCENOBIO¹.

As stated in the previous paper Schenk and Schulz (2015), there is a high potential for saving energy in the process of making wine. In 2009, the energy consumption generated 0.08% of the global greenhouse gas emissions or in other words about 2 kg/0.75l bottle (Smyth et al. (2011)). For instance in California the annual energy requirements of the wine industry are located at 400 GWh. This makes it the second highest energy consumer in the food industry (Galitzky et al. (2005)). Thereby, the control of the fermentation temperature plays a crucial role (Freund (2009); Bystricky (2009); Freund (2008)). Therefore, the minimization of the energy needed for cooling during wine fermentation matters. In Schenk et al. (2014), a novel process model representing the dynamic process of wine fermentation including the yeast dying phase has already been introduced. This model shows the behavior of yeast cells observed in experiments. An illustration of and more information on the yeast growth

phases can be found in Dittrich and Gromann (2011). More-

- *Corresponding author
- ¹RŒNOBIO: Robust energy-optimization of fermentation processes for the production of biogas and wine
 - ²MPC: Model Predictive Control
 - ³ENMPC: Economic Nonlinear Model Predictive Control
 - ⁴PSE: Parameter and State Estimation
 - ⁵SQP: Sequential Quadratic Programming
 - ⁶NMPC: Nonlinear Model Predictive Control
 - ⁷EMPC: Economic Model Predictive Control
 - ⁸PSEP: Parameter and State Estimation Problem
 - ⁹OCP: Optimal Control Problem
 - ¹⁰BDF: Backward Differentiation Formula
 - ¹¹ACADO: Automatic Control and Dynamic Optimization
 - $^{12}\mbox{DLR}$: Dienstleistungzentrum Ländlicher Raum

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over, this model also includes oxygen which is an important factor for yeast activity. A slightly modified version of this model reflects the process of wine fermentation as observed in experiments reduced to the most important substrates involved.

In addition to this, as for the energy-optimal control problem in Schenk and Schulz (2015), for solving a MPC² problem with an objective functional minimizing the energy con-sumption and maintaining the quality of the wine, the tem-perature development has to be added to the model. Sugar being transformed into alcohol is an exothermic reaction. This means that the produced heat has to be dissipated as the temperature development is very important for the yeast. If the fermentation temperature is too high, yeast cells will die. However, in the phase where oxygen is available, even more heat is generated. Moreover, the change of temperature due to the tank's environment and the cooling element which is switched on or off based on the control input are taken into

In this paper, an Economic Nonlinear Model Predictive Control (ENMPC³) problem, minimizing the cooling energy, needed during the fermentation process by controlling the fermentation temperature and maintaining the wine quality (especially of white wine), with the performance of parameter and state estimation (PSE⁴) is solved. This means that whenever new measurements are available the model parameters and states are estimated again and the new control input is computed. The MPC² and PSE⁴ problems are solved by making use of a multiple shooting method (Plitt (1981); Bock and Plitt (1984); Bock (1987)) for the parametrization of the problems and a sequential quadratic programming (SQP⁵) method (as in Nocedal and Wright (2006)) for the solution of the resulting constrained nonlinear optimization problems.

Further information on Nonlinear Model Predictive Control (NMPC⁶) or an introductory overview to the different NMPC⁶ schemes can be found for instance in Allgöwer et al. (1999) and Huba et al. (2011). For NMPC⁶ problems, the objective functions are usually of tracking type. In comparison to NMPC⁶, Economic Model Predictive Control (EMPC⁷) is another type of MPC² with the objective of maximizing the system's profitability, i.e. in our case minimizing the energy consumption. A standard EMPC⁷ formulation can be found for instance in Ellis and Christofides (2015). In this paper, the objective is a combination of both structures, so we study an ENMPC³ problem.

In Section 2, the control system including the model representing the wine fermentation process and its other components like parameter and state estimation and EMPC⁷ are introduced. Then, the methods for solving this control system are presented. In Section 3, the introduced methods are applied to the considered control system. It follows a com-

parison and discussion of the results regarding an industrial control input and our optimal control input. Conclusions are presented in Section 4.

2. Material and methods

2.1. The nonlinear control system

2.1.1. General structure

The entire open-loop nonlinear control system is illustrated in Figure 1. Its components will be described in detail in the following or more precisely in Section 2.1.3 and Section 2.1.4.

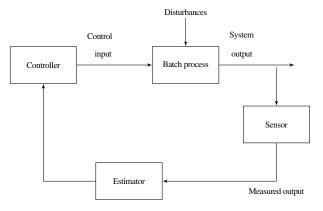


Figure 1: The control scheme

Furthermore, in this paper whenever we talk about the system model, we mean a system of nonlinear ordinary differential equations of the form

$$\dot{x}(t) = f(t, x(t), u(t), d, p)$$

with the differential states represented by x, the control inputs represented by u(t), the unknown disturbances expressed by d and the parameters represented by p. In addition to this, box constraints for all the variables will be allowed.

2.1.2. Process Model Description

First, we introduce a slightly modified version of the model introduced in Schenk et al. (2014) by (1). It represents the process of wine fermentation as it can be observed in real experiments.

Thereby, yeast growth is dependent on the consumption of the nitrogen, sugar and oxygen concentration. Sugar is converted into ethanol but also inhibited by ethanol.

The sugar concentration can be divided into two parts, the amount of sugar for the conversion into ethanol and the amount of sugar which is consumed by the yeast as a nutrient. Furthermore, a process under aerobic conditions

is described by this model as oxygen is an important factor for yeast activity. 142

$$\begin{cases} \frac{dX}{dt} = \mu_{max}(T) \frac{N}{K_N + N} \frac{S}{K_{S_1} + S} \left(\frac{O_2}{K_O + O_2} + \epsilon \right) X \\ -k_d X - \Phi(E) X \end{cases}$$

$$\frac{dN}{dt} = -k_1 \mu_{max}(T) \frac{N}{K_N + N} \frac{S}{K_{S_1} + S} \left(\frac{O_2}{K_O + O_2} + \epsilon \right) X$$

$$\frac{dE}{dt} = \beta_{max}(T) \frac{S}{K_{S_2} + S} \frac{K_E(T)}{K_E(T) + E} X$$

$$\frac{dS}{dt} = -k_2 \frac{dE}{dt}$$

$$-k_3 \mu_{max}(T) \frac{N}{K_N + N} \frac{S}{K_{S_1} + S} \left(\frac{O_2}{K_O + O_2} + \epsilon \right) X$$

$$\frac{dO_2}{dt} = -k_4 \mu_{max}(T) \frac{N}{K_N + N} \frac{S}{K_{S_1} + S} \frac{O_2}{K_O + O_2} X$$

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

The death of yeast cells, due to the accumulation of a high alcohol concentration, which is included in the differential equation for yeast, is described by the following nonlinear term

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

where tol stands for the tolerated ethanol concentration, e.g. tol = 79 g/l which was determined by a set of data produced at Geisenheim University. Moreover, k_{d_1} and k_{d_2} are parameters corresponding to the death of yeast cells due to the exceedance of the ethanol tolerance tol. This death term ensures that the stationary and death phase of yeast cells occur. The evolution of yeast cells in these phases is dependent on the concentration of ethanol. Ethanol inhibits the yeast such that if its concentration is below a tolerance tol the amount of yeast cells stays stationary, and if it exceeds tol, the yeast cells start dying.

The death of yeast cells due to other circumstances is ensured by the second term in the differential equation for the yeast. Thereby, k_d is the parameter corresponding to the part of yeast dying due to other circumstances. This model formulation uses Michaëlis-Menten kinetics. Here, the specific growth rates $\mu_{max}(T)$ and $\beta_{max}(T)$ are linearly dependent on temperature T. Moreover, K_N and K_O are the Michaëlis-Menten half-saturation constants associated to nitrogen or respectively oxygen. Furthermore, $K_E(T)$ represents the temperature dependent ethanol inhibition. The parameters k_1 and k_4 are the yield coefficients 188

associated to nitrogen and respectively oxygen.

In this model, two saturation constants associated to sugar, namely K_{S_1} and K_{S_2} , due to the two parts explained above, are needed. Thereby, K_{S_1} is the saturation constant associated to the part of sugar used for yeast activity and K_{S_2} is the saturation constant associated to the part of sugar needed for the accumulation of alcohol. Furthermore, also two yield coefficients k_2 and k_3 associated to the two different parts of sugar are needed.

The main difference to the process model introduced in Schenk et al. (2014) is the constant ϵ in the oxygen consumption term. This constant was introduced due to the fact that even if there is no oxygen available any more other nutrients are consumed by the yeast for its activity. Due to its introduction, we also have to add another death term, the second term in the yeast equation, to keep the balance in the yeast population.

In case of computing the future control input by solving an optimal control problem several times, the system of differential equations representing the process includes an additional differential equation for the temperature development. This differential equation looks like this

$$\frac{dT}{dt} = \alpha_1 \frac{dE}{dt} - \alpha_2 \frac{dO_2}{dt} - \alpha_3 (T - u_c) \omega_1(t) - \alpha_4 (T - T_{ext}).$$
 (3)

This differential equation for temperature is based on a few assumptions like that with the accumulation of ethanol, the temperature inside the fermentation tank increases and at the beginning where oxygen is still present, even with a higher impact. In equation (3) α_1 expresses how much heat is generated by the conversion of sugar into alcohol. Furthermore, α_2 represents the measure of how the disappearance of oxygen reduces this accumulation of heat. α_3 can be interpreted as a heat transfer coefficient which is the smaller the greater the wine tank in relation to the cooling element is. Furthermore, α_4 can be interpreted as another heat transfer coefficient describing the heat transfer from the exterior of the tank to the interior of the tank. Thereby, T is the current temperature in the fermentation tank and u_c the constant temperature of the cooling fluid flowing through the cooling element. The control input ω_1 determines whether and when cooling shall take place or not.

2.1.3. Parameter and state estimation

As MPC² couples an estimation of the current state and parameters with a receding horizon control of the future, usually for short future time intervals, as a basis, we have to set up and solve a parameter and state estimation problem (PSEP⁸). Thereby, parameters and states are estimated by making use of the past available measurements. The estimated parameters and states for the current point of time are

then used for the model initialization of the EMPC⁷ problem. The PSEP⁸ that has to be solved looks like the following.

$$\min_{x,p} \sum_{i=0}^{N_c} ||\eta_i - g(t_i, x(t_i), d(t_i), p)||_{S_i}^2,$$
s.t. $\dot{x}(t) = f(t, x, d, p), \ t \in [t_0, t_c]$

$$c(x(t_0), ..., x(t_c), p) = 0 \text{ or } \ge 0$$
(4)

with a least-squares objective functional weighted with the positive semi-definite weighting matrices $S_0...S_c$ which are typically the inverses of the variance-covariance matrices related to the measurement errors in our case represented by the mean value of the measurements. The measured data is represented by η_i where these are measurements for the sugar and ethanol concentration at time sample points $t_0...t_c$. Moreover, $g(t_i, x(t_i), d(t_i), p)$ represents the corresponding model output.

The system of differential equations $\dot{x}(t) = f(t,x,d,p)$ refers to system (1) with the differential states $x = (X,N,E,S,O_2)^T$ and parameters p. Furthermore, additional equality and box constraints for the differential states and parameters in this formulation are represented by the function c.

A parameter and state estimation problem is a subclass of ²⁴³ an optimal control problem (OCP⁹) and there are several ²⁴⁴ different ways of solving OCPs as demonstrated in Binder ²⁴⁵ et al. (2001).

For this case, the discretization of the PSEP⁸ (4) was performed making use of a direct multiple shooting approach (Plitt (1981); Bock and Plitt (1984); Bock (1987)), a backward differentiation formula method (BDF¹⁰, as in Hairer (2010)) for the numerical integration of the system of ordinary differential equations and a SQP⁵ method (as in Nocedal and Wright (2006)) for the solution of the resulting constrained nonlinear optimization problem. In detail the solution of this optimization problem is performed as in Schenk and Schulz (2015). All of these methods were implemented using the ACADO¹¹ toolkit - a toolkit for Automatic Control and Dynamic Optimization developed by Moritz Diehl et al Houska et al. (2009–2013).

2.1.4. Economic nonlinear model predictive control

After the basis for the model initialization, the parameter and state estimation using a full information approach, was established in the last section, now, we can take care of the formulation of the ENMPC³ problem. The MPC² procedure is illustrated in Figure 2. At the current state the state and parameters are initialized by making use of the parameter and state estimation based on the past measurements. Now, the future open-loop control input is computed and the future state is predicted by solving the formulated MPC² problem.

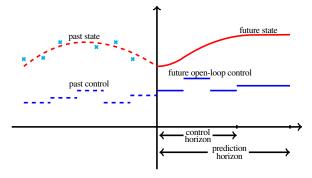


Figure 2: The discrete MPC scheme

Based on the current states $\hat{x}(t_c)$, disturbances \hat{d} and parameter estimates \hat{p} the role of MPC² consists in the prediction of the system's future dynamic behavior and the determination of the future control inputs. This leads to the optimization of an open-loop objective functional over a fixed time horizon \mathcal{T} . However, the system's real behavior deviates from the predicted behavior. This is caused by unknown disturbances and/or due to differences between the model and the dynamics of the real process. Whenever new measurements become available, the new estimates coming from the full information estimation are used, the horizon is shifted and the system's dynamic behavior is predicted from this point of time again. The considered MPC² optimization problem looks like the following

$$\min_{u(\cdot) \in S(\Delta)} \int_{t_c}^{t_c + \mathcal{T}} F(t, x(t), u(t)) dt$$
s.t.
$$\dot{x}(t) = f(t, x(t), u(t), \hat{d}, \hat{p}), \forall t \in [t_c, t_c + \mathcal{T}] \quad (5)$$

$$x(t_c) = \hat{x}(t_c),$$

$$c(t, x(t), u(t), \hat{d}, \hat{p}) \ge 0, \forall t \in [t_c, t_c + \mathcal{T}]$$

where t_c represents the current point of time and the exact formulation of F(t,x(t),u(t)) depends on the case we consider. For an ENMPC³ formulation it consists of the economic stage cost and a tracking term. It is dependent on the target state and the control input determined by the previous calculation. Moreover, the new calculated control input u is an element of $S(\Delta)$, the family of piecewise constant functions with period $\Delta > 0$ where $\Delta := [t_c, t_{c+1}]$. The finite-time prediction horizon is denoted by $[t_c, t_c + \mathcal{T}]$ where \mathcal{T} represents the future time horizon. Furthermore, \hat{x} , \hat{d} and \hat{p} are the current state disturbance and parameter estimates coming from the parameter and state estimation by making use of past measurements for the current point of time t_c . The constraints in the above formulation are system constraints for the input, state and other constraints.

Additional to the formulation (5), one should define a terminal constraint and/or terminal cost in order to ensure theoretical stability. More information on theoretical stability of MPC² can be found in Magni and Scattolini (2004).

 At t_c ENMPC³ receives a state measurement which is used for model initialization. The OCP⁹ is solved for an optimal piecewise input trajectory by using a direct multiple shooting approach in combination with a BDF¹⁰ method and a SQP⁵ method. This solution procedure is similar to the one for the PSEP⁸ in Section 2.1.3 and its implementation was realized using the ACADO¹¹ toolkit as well.

The control input for the first sampling period is sent to the control actuators. At the next sampling time the OCP⁹ is resolved after receiving a new state measurement by shifting the prediction horizon to the future by one sampling period. As mentioned above, the solution procedure for the considered EMPC⁷ optimization problem (5) is similar to the one for the PESP. The system of differential equations $\dot{x}(t) = f(t,x,u,\hat{d},\hat{p})$ corresponds to the system in (1) with an additional differential equation for the temperature evolution introduced in Equation 3 with the differential states $x = (X,N,E,S,O_2,T)^T$ and control ω_1 . Note that x here differs from x in Section 2.1.3 by the temperature variable T.

3. Results and discussion

3.1. Experimental setup







(a) Experimental (b) Cooling brine sup-(c) Cooling aggregate setup of the two ply tanks

Figure 3: Pictures taken at DLR Mosel

The results presented in this section are based on an experiment that was conducted with the facilities of one of our public research partners, DLR¹² (Dienstleistungszentrum Ländlicher Raum) Mosel in Bernkastel-Kues. Two tanks containing 1000 l Riesling must each, which was clarified by sedimentation, were set up for fermentation.

One of them was controlled by an industrial controller (Figure 3a tank on upper left) based on CO_2 measurements, called industrial cooling strategy in the following. All the equipment and controlling software were provided by the industry partner fp-sensor systems. The other tank was controlled by our MPC² controller (Figure 3a tank on upper right) introduced in the previous section.

Furthermore, the oenologist informed us about the target-setting. They wanted to produce an off-dry state wine Riesling containing approximately 18 g/l residual sugar and 12% alcohol. In addition to this at the beginning of fermentation 0.2 g/l ZYMAFLORE X16 wine yeast (Saccharomyces cerevisiae) was added and other nutrients would be added as per specification and demand in the further process of fermentation. Depending on which kind of yeast is used, one also should preferably stick to certain guidelines for the fermentation temperature and the further addition of nutrients. The utilized yeast is known to form strong flavors of peach, white flowers and yellow fruits. They expected the fermentation to last around 20 days with a fermentation rate, or in other words, a must weight loss rate of approximately 10 g/l/d.

The temperature of the cooling brine (Figure 3b), generated by a cooling aggregate (Figure 3c), is hold at 2°C and the temperature of the wine cellar averages 14.5°C.

3.2. Initial parameter and state identification

As a basis for the computation of the future control, we took parameter values obtained from a parameter and state identification conducted for a similar yeast type, i.e. WhiteArome.

However. some parameters were set to literature values (2013). Juschkat for k_{d_1} , k_{d_2} , K_O and k_4 the values were chosen as in Schenk and Schulz (2015) and for the introduced parameters ϵ and k_d reasonable values were selected (see Table 1). The rest of the model parameters was

Parameters	set
K_N	0.1156
k_1	0.0536
K_{S_2}	4.3262
K_{E_1}	0.2616
K_{E_2}	38.90
k_{d_1}	99.86
k_{d_2}	0.0021
K_O	0.0007
k_4	0.0025
ϵ	0.02
k_d	0.01
tol	79.0

parameters was Table 1: Fixed parameter values estimated as explained above (see Table 2).

Parameters	initial	estimated
μ_1	0.08	0.0514
μ_2	0.1858	4.9325
K_{S_1}	33.35	34.2695
β_1	0.3371	0.3954
β_2	0.0285	0.0
k_2	1.2	1.5324
k ₃	15	15.75

Table 2: Initial parameter estimates

 The fit to sugar measurement data for the similar yeast type and the development is illustrated in Figure 4. Thereby, the simulation output which provides the best fit to the sugar measurements, is illustrated in blue and the linear function expressing the must weight loss rate is represented in pink. The state trajectories show the behavior also observed in real experiments.

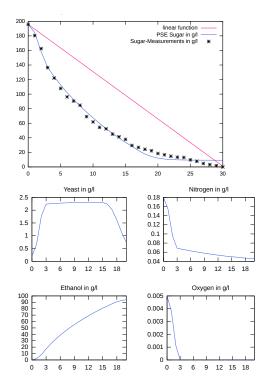


Figure 4: Basic parameter estimation results for similar yeast type

3.3. Economic nonlinear model predictive control

As already mentioned, in industry the main goal consists in maximizing the gain of a product which can be achieved by reducing its production costs without sacrificing its quality. Thus, our objective in the optimization problem, formulated in the following, consists in the minimization of the energy, needed for cooling by controlling the fermentation temperature, in combination with the maintenance of the quality and constraints on the maximum temperature, the control input ω_1 and the residual sugar, expressed by a boundary condition. The considered optimization problem looks like the following

$$\begin{cases} \min_{x,u} \gamma_1 \int_{t_c}^{t_c + T} \omega_1(t) u_c dt + \gamma_2 \int_{t_c}^{t_c + T} (S(t) - \hat{S}(t))^2 dt \\ \text{s.t. } \dot{x}(t) = f(t, x, d, p) \text{ (Process model (1))} \\ \frac{dT}{dt} = \alpha_1 \frac{dE}{dt} - \alpha_2 \frac{dO_2}{dt} - \alpha_3 (T - u_c) \omega_1(t) - \alpha_4 (T - T_{ext}) \end{cases}$$
(6)

with adequate initial values, box constraints and a boundary condition regarding the final sugar concentration, i.e.

$$S_{end} = 18.$$
 (7)

This boundary condition guarantees that the product is going to be an off-dry wine with 18g/l residual sugar. The formulation (6) is an extension of the one in Schenk and Schulz (2015). Thereby, we reformulated the problem introduced in Schenk and Schulz (2015) by using an outer convexification formulation (as first presented in Sager (2005) or later in Kirches (2010)). This reformulation was necessary due to the fact of working with a discrete switching structure for the cooling element which is either turned on or off.

Thereby, \mathcal{T} represents the shrinking time horizon with a fixed end point. Within the objective function formulation the first term represents the energy consumption due to cooling by temperature control and the second term serves the maintenance of the quality assured by consideration of the fermentation rate (must weight loss rate), i.e. $\hat{S}(t) = \frac{S_f - S_0}{t_f - t_0}t + S_0$. This ensures that the sugar is consumed as linearly as possible. For the temperature T and the control input ω_1 , box constraints of the following form

$$13^{\circ}\text{C} \leq T \leq 20^{\circ}\text{C}, \qquad 0 \leq \omega_1 \leq 1$$

are implemented.

The process model and the additional differential equation for the temperature development were already explained in detail in Section 2.1.2. The additional parameters are illustrated in Table 3. They were set to certain values

set
14.5
2
$\frac{21.44}{95}$
1.0
0.1584
0.0434

Table 3: Additional parameter values for the corresponding model

depending on the framework of the experiment like for example the heat coefficient α_1 which is dependent on the accumulation of alcohol. It was calculated based on how much heat is produced by the fermentation of a must which contains 205.3 g/l of sugar. According to Dittrich and Gromann (2011), the fermentation of one mol hexose (≈ 180 g) computes approximately 23.5 kcal/l of heat. This means that if the fermentation process starts with a must of 14°C it can heat up to 35.44°C as around 20% is dissipated with the disappearance of the fermentation gas. This leads to 21.44°C relative to the desired alcohol concentration at the end of the fermentation process for α_1 . α_3 , the convection heat transfer with respect to the cooling jacket,

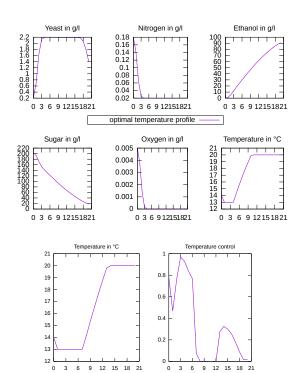


Figure 5: Future open-loop control trajectories for whole horizon with an initial nutrient concentration of 0.18g/l

was assumed to have an impact factor of 0.15841 and α_4 , the convection heat transfer with respect to the exterior of the tank, was set to 0.0434. The rest of the parameters was set to certain values based on experience.

For the differential states, the initial values illustrated in Table 4 were chosen.

<i>X</i> (0)	0.2 g/l
N(0)	0.18 or respectively 0.105 g/l
E(0)	0 g/l
S(0)	205.3 g/l
$O_2(0)$	0.005 g/l
T(0)	14.0° C

Table 4: Initial values for differential states for optimal control problem

Thereby, some of them were measured, like sugar, alcohol 431 and nitrogen and others, like nitrogen for the first computation of the control input, and oxygen were set to these values based on experience. 432

For the first computation of the control input we receive the results illustrated in Figure 5. The predicted trajectories of the product and the substrates represent the behavior also observed in real experiments. The corresponding future tem-

perature profile proceeds in the way that the temperature is supposed to be down-regulated just after the start of fermentation and then after day four the fermentation temperature should be increased linearly up to 20°C at which the fermentation is supposed to be phased out until the aspired residual sugar concentration is reached. The corresponding control input to this temperature behavior shows a similar behavior. After the fermentation process was already running a while, the measured sugar and alcohol concentrations were taken to run a full information estimation of the state and parameters and compute a new future control input. The corresponding results are described by Figure 6. Thereby, the pink line illustrates the linear function representing the must weight loss rate.

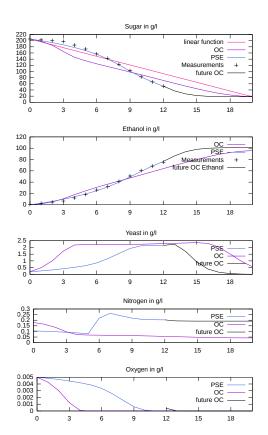


Figure 6: Status during running fermentation process and future prediction

At the top the fit of the simulation to the sugar and alcohol measurements (blue) with the trajectory for the future control input from the current point of time (black) is illustrated and compared to the first predicted state trajectory (purple). They are different from each other for the whole time horizon, the past and future time domain. At the bottom the trajectories resulting from the estimation with the currently predicted trajectories and the first predicted trajectories are

 compared. They differ from each other for the whole time horizon as well. An important point is the addition of nitrogen after day five, handled as a disturbance in the system model, which can be spotted in this graphic.

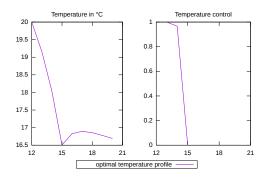


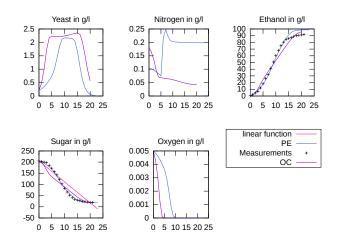
Figure 7: Future open-loop control after day 12

The future open-loop control of the fermentation temperature after day 12 is illustrated in Figure 7. Interpreting the results in detail, in particular the model calibration, showed that the weight for the sugar term has to be adjusted. So for the computation of the control input for the rest of the fermentation process, a new distribution of the weights in the objective functional and a new fermentation rate for the rest of the fermentation were established. The future control input for the new formulation proposed that from now on cooling down is the best option.

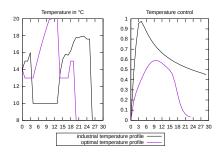
As the produced wine is supposed to be used and it does not just serve experimental purposes, the knowledge and 473 experience of the wine expert is also of high importance. 474 The wine expert decided to cool down even more to be safe. 475 The fermentation process was stopped when the aspired 476 sugar concentration was reached by setting a permanent 477 temperature of 8° C (permanent cooling). 478

After the execution of the experiment, the model was calibrated again. Figure 8a shows a comparison of the state trajectories for the first computed control input (purple) and for the model calibration (blue). The cooling strategy in case of using MPC² (blue) was compared to an industrial cooling strategy (black) which is visualized in Figure 8b. As earlier in this section, the linear function representing the must weight loss rate is visualized in pink.

The energy consumption in case of using the optimal control input equals 17.65 compared to 36.70 in case of using the industrial control input. This means that by using the computed MPC² input the cooling costs can be reduced (in this experiment by approximately 52%).



(a) Comparison of true, estimated and predicted states



(b) MPC²-input vs. industrial control input

Figure 8: Whole trajectories for states and control

All in all, it can be said that the best choice would have been the direct connection of sensors and actuators with MPC^2 controlling software but at this time it was not possible. The major problem is due to the fact that an experiment in this scope is possible only once a year and that we need at least this amount of must for the industrial controlling software to work reliably.

Summing up, we can say that two different cooling strategies were carried out, one where the fermentation is run early at high temperatures and another one where the fermentation is carried out early at low temperatures. As a result, we received two different wine flavor styles, i.e. yellow fruit aroma (classic Riesling taste) for the MPC² strategy and gummy bear/ice candy aroma for the industrial strategy but most notably no off-flavors were formed. Both flavor styles were built from the same yeast but different fermentation temperatures. The MPC² strategy which reached high temperatures early had an advantage for the end of the fermentation regarding the energy consumption. Usually,

the cooling is turned off too late and the exchange with the exterior of the tank is not sufficiently used which can also be observed in this experiment comparing the two different strategies. The MPC² strategy exploits the cooling by the exterior of the tank to save energy by turning off the cooling carried out by the cooling jacket.

4. Conclusions

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In this research article, economic model predictive control with state and parameter estimation for the process of wine fermentation was studied. After a short introduction into the general structure of the optimization procedure, the underlying reaction model and additional differential equations, the methodology namely performing economic nonlinear model predictive control with parameter and state estimation as a basis for the current state was explained in detail. 558 The elaborated methods were applied to a real experiment conducted at the DLR¹² Mosel in Bernkastel. Thereby, two different controllers were used for the control of the fermentation temperature. The results regarding the two different control inputs, one imposed by an industrial controller, another one by making use of the control input computed by solving the ENMPC³ problem, were used. Thereby, an optimal control problem for the minimization of the energy needed for cooling during fermentation in combination with the maintenance of the quality of the wine was set up. All in all, by using the calculated control input from an ENMPC³like strategy the energy consumption can be reduced (in this experiment by approximately 52%). No off-flavors were formed and both wines are tasty.

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