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 using multiple experiments and a comparison of results for a common temperature profile and an optimal temperature profile in Section 5. Conclusions are presented in Section 6.

2. PROCESS MODEL DESCRIPTION

First, we recall the model introduced in Borzì et al. (2014). It describes the wine fermentation process as it can be observed in real experiments.

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

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 model because it plays a crucial role for yeast activity, especially in the case of using a Saccharomyces cerivisae yeast strain.
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 with simultaneous maintenance of the quality of the product. This is what we take as our objective in the formulated OCP, namely the goal is to reduce the energy needed for cooling by controlling the fermentation temperature.
This means that temperature is the degree of freedom in the considered OCP.
Thereby a certain final ethanol concentration is aspired which is expressed by a boundary condition (equation (17)).

$$
\begin{aligned}
&\min J(u) := \int_0^{t_f} |T_{ext} - u(t)| dt \\
&\text{s.t.} \\
&\begin{cases}
\text{Model (1)} \\
\frac{\partial T}{\partial t} = \alpha_1\frac{\partial E}{\partial t} - \alpha_2\frac{\partial O_2}{\partial t} - \alpha_3(T - u)
\end{cases}
\end{aligned}
\tag{3}
$$

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 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 parameter estimation problem

(4) and of the optimal control problem (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); Houska et al. (2009–2013)).
The application of these methods to our problems is described in detail in the following two subsections.

4.1 Parameter Identification

The process model (1) contains many parameters. These parameters have to be identified.
The parameter estimation problem that has to be solved looks like the following.

$$\begin{aligned}
&\min_{y,p} r_1(y(t_0), ..., y(t_N), p) \\
&= \min_{y,p} \sum_{i=0}^{N} \frac{(\eta_i - g(t_i, y(t_i), p))^2}{\sigma_i^2} \\
&\text{s.t.} \\
&\begin{cases} \dot{y}(t) = f(t, y, p), \quad t \in [t_0, t_N] \\ \underline{r} \le r_2(y(t_0), \ldots, y(t_N), p) \le \bar{r} \end{cases}
\end{aligned} \tag{4}$$

with a least-squares objective functional minimizing the sum of squares of the weighted residuals represented by the estimating function r_1. The measured data is represented by η_i where these are measurements for the sugar concentration at time sample points $t_0 \ldots t_N$. σ_i^2 are the variances of the measurements. Here, they are assumed to be the mean values of the measurements. Moreover, $g(t_i, y(t_i), p)$ represents the corresponding model output.
The system of differential equations $\dot{y}(t) = f(t, y, p)$ refers to system (1) with the differential states $y = (X, N, E, S, O_2)^T$ and parameters p, displayed in Table 2. Furthermore, additional equality and box constraints for the differential states and parameters in this formulation are represented by the function r_2.
In detail the process for solving this problem looks like the following.

a) Discretize the boundary value problem by multiple shooting method (see Bock (1987) for further information):
For $i = 0, \ldots N-1$ do

   (i) Discretize state piecewise
   $$y(t) := s_i \quad \text{for } t \in [t_i, t_{i+1}] \tag{5}$$
   (ii) Solve system of ODEs on each interval $[t_i, t_{i+1}]$ numerically (BDF-method) with an initial value s_i
   $$\begin{aligned} &\dot{y_i}(t; s_i, p) = f(y_i(t; s_i, p), p), \quad t \in [t_i, t_{i+1}] \\ &y_i(t_i, s_i, p) = s_i, \end{aligned} \tag{6}$$

end

b) Solve constrained nonlinear least squares problem (7) by SQP method using a stucture-exploiting Broyden-Fletcher-Goldfarb-Shanno (BFGS) update for the approximation of the Hessian.

$$\begin{aligned}
&\min_{s,p} \sum_{i=0}^{N} \frac{(\eta_i - g(t_i, y(t_i; s_i, p), p))^2}{\sigma_i^2} \\
&s.t.\ s_0 - y_0 = 0 \\
&\quad s_{i+1} - y_i(t_{i+1}, s_i, p) = 0, \quad i = 0, \ldots N-1 \\
&\quad \underline{r} \le r_2(s_i, p) \le \bar{r}, \quad i = 0, \ldots, N
\end{aligned} \tag{7}$$

In order to evaluate the quality of our estimate, the variance-covariance matrices have to be calculated. Therefor a linear approximation in the optimal solution is derived. Further information on this procedure can be found in Bock (1987).

4.2 Optimal Control

After the derivation of the optimal control problem and the estimation of most of the parameters involved, this section focuses on the solution of this problem.
The procedure for solving OCP (3) works basically like solving the parameter estimation problem (4) in the last subsection. The system of differential equations $\dot{y}(t) = f(t, y, u)$ corresponds to the system in (3) with the differential states $y = (X, N, E, S, O_2, T)^T$ and control u. Note that y here differs from y in section 4.1 by the temperature variable T.
In detail the solution process looks like the following.

a) Discretize the boundary value problem by multiple shooting method (see Bock (1987) for further information):
For $i = 0, \ldots N-1$ do

   (i) Discretize control piecewise constant
   $$u(t) := q_i \quad \text{for} \quad t \in [t_i, t_{i+1}] \tag{8}$$
   (ii) Solve system of ODEs on each interval $[t_i, t_{i+1}]$ numerically (BDF-method) with an initial value s_i
   $$\begin{aligned} &\dot{y_i}(t; s_i, q_i) = f(y_i(t; s_i, q_i), q_i), \quad t \in [t_i, t_{i+1}] \\ &y_i(t_i, s_i, q_i) = s_i, \end{aligned} \tag{9}$$
   (iii) Numerically compute integrals (objective functional in Lagrange form)
   $$l_i(s_i, q_i) := \int_{t_i}^{t_{i+1}} L(y_i(t_i, s_i, q_i), q_i)dt \tag{10}$$

end

b) Solve nonlinear constrained optimization problem (11) by SQP method using a stucture-exploiting BFGS update for the approximation of the Hessian.

$$\begin{aligned}
&\min_{s,q} \sum_{i=0}^{N-1} l_i(s_i, q_i) \\
&s.t.\ s_0 - y_0 = 0 \\
&\quad s_{i+1} - y_i(t_{i+1}, s_i, q_i) = 0, \quad i = 0, \ldots N-1 \\
&\quad \underline{c} \le c(s_i, q_i) \le \bar{c}, \quad i = 0, \ldots, N \\
&\quad \underline{E} \le r(s_N) \le \bar{E}
\end{aligned} \tag{11}$$

Thereby, c is the function of box constraints for the differential states and the control and r corresponds to the boundary condition, in form of a box constraint, regarding the final ethanol concentration.

5. NUMERICAL RESULTS

In this section numerical results applying the methods introduced in the latter section to our process model are presented. All the results shown in this section were obtained by using the ACADO toolkit - a toolkit for Automatic Control and Dynamic Optimization developed by Moritz Diehl et al. (Ariens et al. (2010–2011); Houska et al. (2009–2013)).

5.1 Parameter Identification

At first, results concerning the estimation of the involved parameters are visualized.
One of our industry partners, DLR Mosel, provided us with measurements of Oechsle values. To render them useful for our model (1) we assumed that 1°Oechsle corresponds to a sugar concentration of 2.2 g/l. As one set of these measurements was not sufficient for estimating the parameters, we moved on to run multiple experiments. For the differential states the initial values illustrated in Table (1) were chosen.
In addition to this, we set box constraints for most of the

$X(0)$	0.2 g/l ($\approx 400000/ml$)
$N(0)$	0.17 g/l
$E(0)$	0 g/l
$O_2(0)$	0.005 g/l

Table 1. Initial values for differential states for parameter estimation problem

differential states based on experience, i.e.

$$\begin{aligned} 0 \text{ g/l} \leq & N \leq 0.17 \text{ g/l}, \\ 0 \text{ g/l} \leq & E \leq 100 \text{ g/l}, \\ 0 \text{ g/l} \leq & S \leq 213.4 \text{ g/l}, \\ & \text{and} \\ 0 \text{ g/l} \leq & O_2 \leq 0.005 \text{ g/l}. \end{aligned} \tag{12}$$

The maximum specific growth rates $\mu_{max}(T)$ and $\beta_{max}(T)$ and the inhibition rate $K_E(T)$ were assumed to be linear dependent on temperature such that

$$\begin{aligned} \mu_{max}(T) &= \mu_1 T - \mu_2, \\ \beta_{max}(T) &= \beta_1 T - \beta_2 \\ & \text{and} \\ K_E(T) &= -K_{E_1} T + K_{E_2} \end{aligned} \tag{13}$$

where for the temperature T a linear temperature profile was chosen. This means T equals 15°C for the first half of the fermentation, 18°C for the second half of the fermentation and it exists a linear ascent in between.
The upper and lower bounds of the parameters p were selected dependent on the initial guesses p_{init}, i.e.

$$(1 - l_b) p_{init} \leq p \leq (1 + u_b) p_{init} \tag{14}$$

where l_b was chosen to be equal to 1 and u_b was chosen to be equal to 7.
For the case of using two sets of measured data, the results for fitting the model are visualized in Figure 1 and Table 2.
It is visible that for these two similar courses of sugar

Parameters	initial	estimated
μ_1	0.0210	0.1681
μ_2	0.1858	0.0
K_N	0.0925	0.1096
k_1	0.7	0.0720
K_{S_1}	33.35	29.5
K_{S_2}	4.3	7.081
K_{E_1}	0.2616	0.0
K_{E_2}	38.90	85.73
β_1	0.0337	0.2696
β_2	0.2855	0.0
k_{d_1}	100	99.86
k_{d_2}	0.003	0.0021
k_3	1.5	12.0
K_O	0.001 25	0.0038
k_4	1.05	0.0019

Table 2. Parameter estimates

measurements a good fit was obtained.
However, the question is whether it is also a good estimate. That is why we examine the degree of uncertainty of the parameter estimation. So, we take a look at the standard deviations of the parameters or respectively the square roots of the diagonal elements of the variance covariance matrix.

$$\begin{array}{llr} \mu_1 = 0.1681 & \pm\ 0.0 & 0\% \\ \mu_2 = 0.0 & \pm\ 0.0 & 0\% \\ K_N = 0.1096 & \pm\ 0.01651 & 15.1\% \\ k_1 = 0.07199 & \pm\ 0.01162 & 16.1\% \\ K_{S_1} = 29.5 & \pm\ 0.4038 & 1.4\% \\ K_{S_2} = 7.081 & \pm\ 12.07 & 170.5\% \\ K_{E_1} = 0.0 & \pm\ 0.0 & 0\% \\ K_{E_2} = 85.73 & \pm\ 3.337 & 3.9\% \\ \beta_1 = 0.2696 & \pm\ 0.0 & 0\% \\ \beta_2 = 0.0 & \pm\ 0.0 & 0\% \\ k_{d_1} = 99.86 & \pm\ 0.1578 & 0.2\% \\ k_{d_2} = 0.002059 & \pm\ 0.005696 & 276.6\% \\ k_3 = 12.00 & \pm\ 0.0 & 0\% \\ k_4 = 0.001868 & \pm\ 0.0001837 & 9.8\% \\ K_O = 0.003759 & \pm\ 0.001477 & 39.2\% \end{array} \tag{15}$$

These confidence intervals of the parameters show that some of them are large or even very large. This means that these parameters are poorly determined. Nevertheless, there are other parameters like for example μ_1 which are determined really well.

5.2 Optimal Control

In the following, numerical results regarding the solution of the given OCP are compared to the trajectories associated with a temperature profile as it is common to use in wine industry.
An optimal solution to the OCP (3) was generated. For the parameters involved, the values displayed in Table 2 and Table 3 were used. Most of the parameters come from the parameter estimation whose results were presented in the latter subsection. However, k_4 and K_O were set

Parameters	set
K_O	0.0007
k_4	0.0025
k_2	2.1544
T_{ext}	15.0
K_{O_2}	0.0004
tol	70.0
α_1	$\frac{22.3}{85}$
α_2	1.0
α_3	0.15

Table 3. Additional parameter values for the corresponding model

$X(0)$	0.2 g/l ($\approx 400000/ml$)
$N(0)$	0.17 g/l
$E(0)$	0 g/l
$S(0)$	213.4 g/l
$O_2(0)$	0.005 g/l
$T(0)$	15.0 °C

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

to different values as they were estimated because the concentration of oxygen has to totally disappear faster than what came out by using their estimates. The other parameters were set to certain values 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 213.4 g/l of sugar. According to Dittrich and Gromann (2011), the fermentation of one mol hexose ($\approx$ 180 g) computes approximately 23.5 kcal/l of heat. This means that if the fermentation process starts with a must of 15°C it can heat up to 37.3°C as around 20% is dissipated with the disappearance of the fermentation gas. This leads to 22.3°C relative to the minimum achieved alcohol concentration at the end of the fermentation process for α_1. 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.

Furthermore, we set box constraints for most of the differential states based on experience, like in (12). The maximum specific growth rates $\mu_{max}(T)$ and $\beta_{max}(T)$ and the inhibition rate $K_E(T)$ were assumed to be linear dependent on temperature like in (13). For temperature T and control u we considered box constraints of the following form

$$\begin{aligned} 15°\mathrm{C} \leq & T \leq 20°\mathrm{C} \\ 0°\mathrm{C} \leq & u \leq 25°\mathrm{C} \end{aligned} \tag{16}$$

in accordance with the knowledge of how much heat is produced which was mentioned above.

Moreover, the alcohol concentration at the end of fermentation is supposed to be located between 85 and 90 g/l, i.e.

$$85 \text{ g/l} \leq E(t_f) \leq 90 \text{ g/l}. \tag{17}$$

Under these circumstances, using the methods described in the latter section, the algorithm converges after 854 iterations, with a KKT-tolerance of 4.995×10^{-5} and 36 time intervals chosen for the discretization, and the results represented in Figure 2 are obtained, where a standard (blue) and optimized (red) temperature profile are compared.

The trajectories of the product and the substrates for the two different temperature profiles look very similar but for the optimal profile the sugar is consumed faster. Therefore the aspired ethanol concentration is reached sooner and the yeast cells start dying sooner.

In the main phase of fermentation the temperature rises to its upper bound and decreases when the aspired final ethanol concentration is reached. For the corresponding control, we can say that at the beginning where oxygen is still present but not much alcohol yet, the cooling temperature does not need to be low yet. With the absence of oxygen, the temperature of the fluid that flows through the cooling element becomes cooler. Compared to this, the control associated with the common temperature profile rises almost linear.

The objective function value for the optimal control profile equals 55.69 compared to 124.62 for the usual control. This means that by using the new optimal profile the cooling costs can be reduced by approximately 55%.

6. CONCLUSION

In this work, parameter estimation for a model describing the wine fermentation process including the yeast dying phase was conducted. Moreover, the parameter estimates were evaluated regarding their quality. By making use of these identified parameters an energy-optimal control problem controlling the fermentation temperature was solved. The we compared the trajectories for the resulting optimal control profile to the use of a standard profile, as it is common to use in the industry of making wine. All in all, the energy consumption using the optimal control profile for controlling the temperature of the fermentation process could be reduced by 55%.

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Appendix A. ADDITIONAL FIGURES

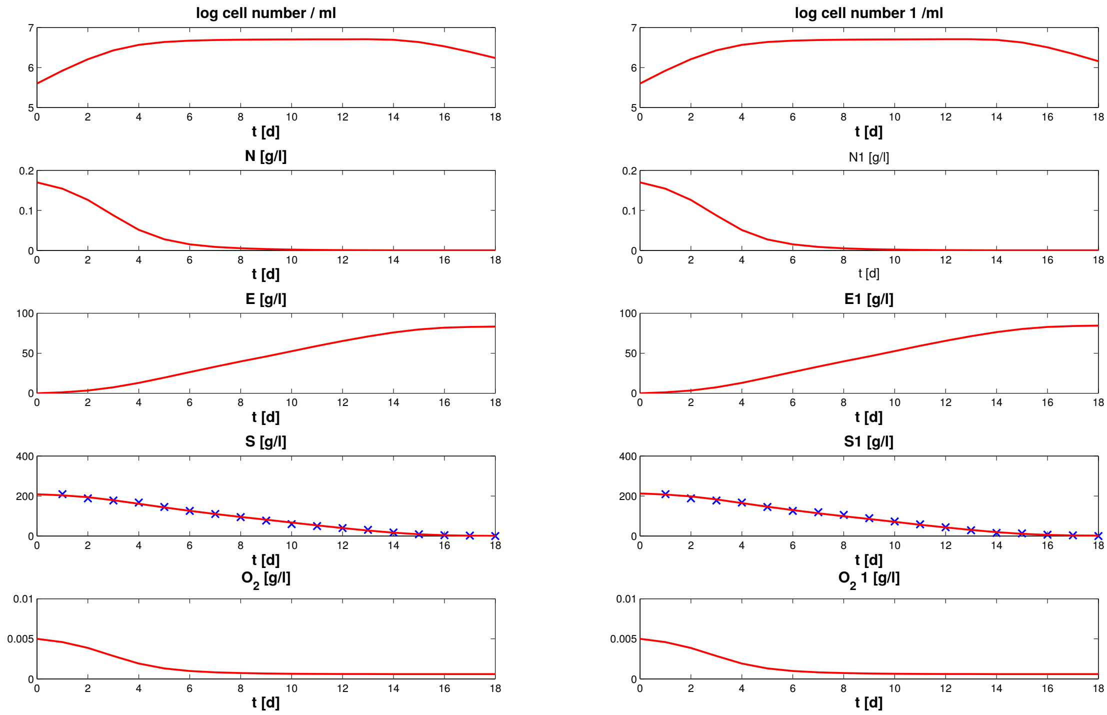

Fig. 1. Fit (red) for two similar sets of sugar concentration measurements (blue)

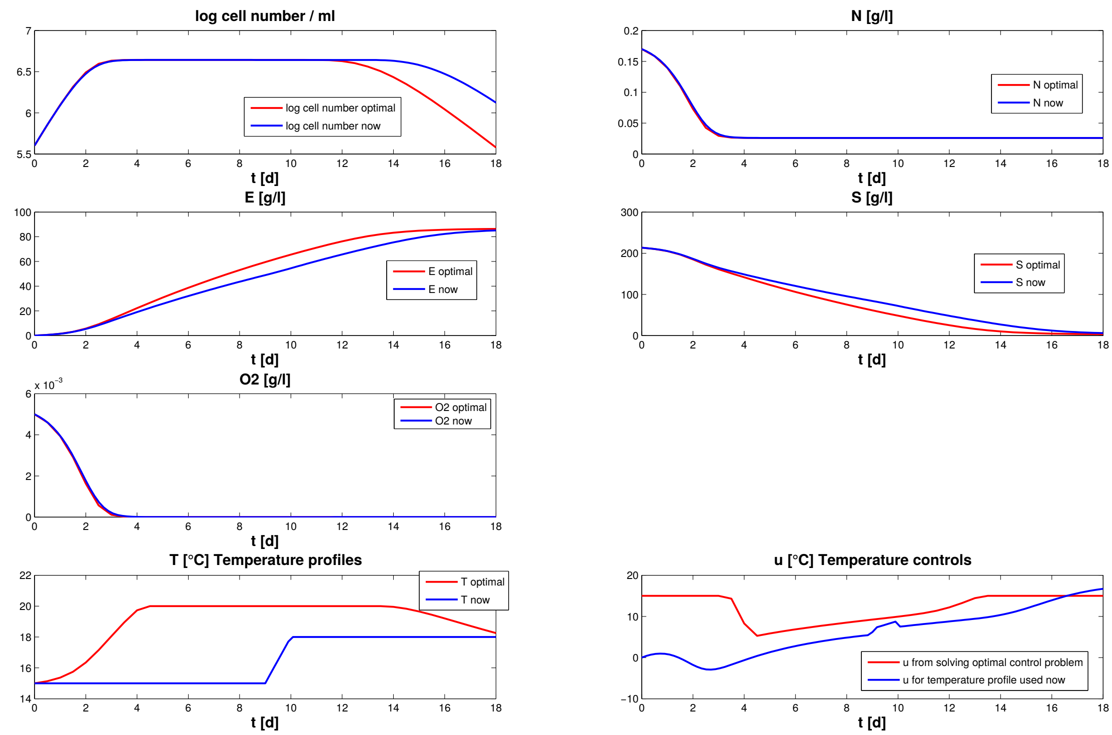

Fig. 2. Comparison of standard (blue) and optimized (red) temperature profile

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