SIMULATION AND OPTIMIZATION OF ALCOHOLIC FERMENTATION IN WINEMAKING

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Abstract. Alcoholic fermentation is an important step of wine making process. Automatic techniques using on line monitoring of fermentation, modelling and process optimisation would be a valuable new instrument for winemakers. In fact, the fermentation duration and the total energy required for temperature regulation could be predicted and optimised, not only in one tank but also in the whole winery.

We proposed a dynamic model of alcoholic fermentation based on the main yeast physiological mechanisms. This model consists of ordinary differential equations including numerous parameters that need to be identified and important interactions between explanatory variables. The model predicted accurately the fermentation kinetics of >80% of a large number of experiments performed with 20 wine yeast strains, 69 musts and different fermentation conditions.Thanks to the wide domain of validity of the model, a simulator based on this model was developed to help winemakers to optimize tank management. It not only predicts the end of the fermentation and changes in the rate of fermentation, but also includes an optimization module based on fuzzy logic. Optimized temperature profiles and nitrogen addition strategies are proposed to decrease the duration of fermentation and energy requirements at winery scale, according to user specifications.

Introduction

Alcoholic fermentation is an important step of wine making process. During alcoholic fermentation, hexoses are converted to ethanol and carbon dioxide, but many other compounds are removed from the must and a large set of by-products are formed that affect the sensorial properties of the wine. Optimising the control of alcoholic fermentations for winemaking is a difficult challenge. Unlike some other kinds of industrial fermentations, such fermentations do not aim to maximise the concentration or yield of a defined metabolite, or the productivity of the process. In winemaking, the main objective is to optimise product quality, which is very difficult to quantify, but the control of technological parameters, such as sugar exhaustion, fermentation duration and the amount of energy required to regulate temperature is also of interest. Many works have shown that fast fermentations may be detrimental to the quality of the wine, especially for white wines. Therefore it is important to control, as far as possible, the duration of the fermentation. Too long a fermentation not only delays the subsequent processes but also increases the risks of wine damage. Control over fermentation kinetics generally has direct technological advantages, in terms of tank use optimization in the winery and control over energy expenses for the regulation of temperature. It is generally a prerequisite for controlling the characteristics of the wine.

We proposed a dynamic model of alcoholic fermentation based on the main yeast physiological mechanisms [7]. We then elaborated a thermal model to calculate the amount of energy produced by the fermentation. Consequently the models can predict the evolution of temperature inside the tank and/or the power consumption for temperature regulation [3]. Finally, we designed a simulator to help winemakers to optimise tank management [6]. It predicts the end of the fermentation and changes in the rate of fermentation and it includes a decision support module based on fuzzy logic. Optimized temperature profiles and nitrogen addition strategies are proposed to decrease the duration of fermentation and energy requirements at winery scale, according to user defined specifications.

1 Models

1.1. Kinetic model

The kinetic model is based on the main physiological mechanisms limiting the yeast activity. To assess its interest in the practice, we tested it in many different winemaking conditions.

1.1.1 Model structure

In this model, yeast activity is implicitly described by four subsystems: (a) glucose transport, inhibited by ethanol *E(t)* and the limiting feature of fermentation [7], described by the function v_{ST}; (b) glycolysis, *i.e.* glucose degradation into ethanol and CO_2, which is not limiting; (c) nitrogen transport, also strongly inhibited by ethanol, described by the function v_N; and (d) the synthesis of glucose transporters from a fraction of the absorbed nitrogen, modeled by the function N_{ST}. The model predicts the speed at which glucose is consumed, and the amount of ethanol or CO_2 produced. It includes the effects of the main involved factors: temperature *T(t)*, which can vary within a predefined range and assimilable nitrogen *N(t)*, which has a major impact on the yeast activity and varies a lot according to the musts.

The model is described by the following differential equations:

$$\begin{cases} \frac{dS}{dt} = -X(t)\ v_{ST}(S(t),E(t),T(t))\ N_{ST}(N_{\max}(t)-N(t),X(t),T_{ucd}(t)), & S(0)=S_{init} \\ \frac{dN}{dt} = -X(t)\ v_{N}(N(t),E(t),T(t)), & N(0)=N_{\text{init}} \\ \frac{dX}{dt} = \mu(T(t))\ X(t)\ (1-\frac{X(t)}{X_{\max}(N_{init})}), & X(0)=X_{init} \end{cases} \quad (1)$$

with T_{ucd} the temperature to the end of the growth phase, $\text{Nmax}(t)=N_{init}+N_{add}(t)$, N_{add} being the amount of nitrogen added, if any.

Assuming Gay-Lussac-like relationships, the concentrations of glucose *S(t)* and ethanol *E*(*t*), together with *dS/dt* and *dE/dt*, can be deduced from the amount of carbon dioxide released, $CO_2(t)$, using equation (2) [5]:

$$\begin{cases} S(t) = S_{init} - 2.17\ \mathrm{CO}_2(t), & \mathrm{CO}_2(0) = 0 \\ E(t) = 0.464(S_{init} - S(t)). \end{cases} \quad (2)$$

The model takes into account both yeast growth, equal to *X(t),* and the average activity of a single yeast cell in its environment, equal to $v_{ST} * N_{ST}$. The cell growth model is a logistic model, given in its differential form in equation (1), where $\mu(T(t))$ represents the specific growth rate.

1.1.2 Model validity

Colombié *et al.* [2] tested the model in various conditions, including anisothermal studies and additions of ammoniacal nitrogen. The tests covered synthetic media and natural musts corresponding to 25 varieties from 6 French vine-growing area. Twenty different commercial yeast strains were used. The average prediction error on the fermentation duration was less than 10 %, except for sluggish fermentations, which could not be accurately predicted. Therefore the model has a sufficiently large domain of validity to be of potential interest for practical use.

	Synthetic media	Natural musts (classical fermentations)	Natural musts (sluggish fermentations)	Yeast strains
Number of experiments	23	46	15	20
E_d (%)	9.1	8.5	24.3	8.5

Table 1. Comparison of simulated and experimental fermentation kinetics of experiments performed with different synthetic and natural media and with different yeast strains. *E_d* = |*Dexp – Dsim* | / *Dsim* (error on fermentation duration)

1.2 Thermal model

1.2.1 Model structure

Colombié *et al.* [3] developed a model for calculating heat transfer in tanks during fermentation. This model is based on the transient equation for power conservation:

$$P_{accumulation}(t)=P_{fermentation}(t) - P_{wall}(t) - P_{evaporation}(t) - Q_c(t), \quad (3)$$

with $P_{fermentation}$ the power generated by the fermentation, $P_{accumulation}$ the power accumulated by the must, P_{wall} the power exchanged by convection through the tank wall, $P_{evaporation}$ the power lost through evaporation and Q_c the power required to cool the tank.

$$P_{accumulation}(t)=10^{-3}\ \rho_{must}\ VCp_{must}\ \frac{dT}{dt}, \quad (4)$$

where ρ_{must} is the must density, *V* the tank volume and Cp_{must} the specific heat of the must in fermentation.

$$P_{fermentation}(t) = \frac{23500 * 2.17}{180} V \frac{dCO_2}{dt}, \quad (5)$$

$$P_{wall}(t)=10^{-3}\ UA\ (T(t)-Te(t)), \quad (6)$$

where A is the exchange area, Te the air temperature and U is the overall heat transfer coefficient, $U = \frac{1}{\frac{1}{hi} + \frac{1}{he} + \frac{e}{\lambda}}$, hi and he are the convection coefficients at the inside and the outside surface of the tank respectively, e is the thickness of the tank material and λ is the thermal conductivity of the tank material.

$$P_{evaporation}(t) = \frac{0.2233V \frac{dCO_2}{dt}(2 + \frac{10.85CO2}{1514.19 - 0.95(S0 - 2.17CO2)}1.0592^{T}}{270.92 - (2 + \frac{10.85CO_2}{1514.19 - 0.95(S_0 - 2.17CO_2)}1.0592^{T}} \quad (7)$$

1.2.2 Model validation

The model was validated by Colombié et al. [2] at the pilot scale (100 liter tanks), using two different methods. The authors compared the experimental CO_2 production and the predicted one using the kinetic model [7] and the thermal one. The difference between the calculated temperature and the experimental one remained lower than 1°C throughout the fermentation. The thermal model was not tested for large tanks for which the surface area to volume ratio is small. In this case, the heat loss through convection represents only a small percentage of the heat produced by the fermentation (less than 10%). Thus we may reasonably assume that the model is applicable at industrial scale.

1.3 Global model

From the definition of $P_{accumulation}(t)$ in equation (4), we remark that the transient equation for power conservation (3) is actually a dynamic model describing the temperature evolution dT/dt within the must. This equation is connected to the kinetic model (1)-(2). The whole system composed from equations (1) to (7) has been considered for optimization purposes. It is a complex controlled dynamical system, whose control variables are cooling power Q_c and nitrogen addition. Note also that the temperature T is constrained in a fixed range: $T_{min} \leq T \leq T_{max}$.

2 Optimization

2.1 Optimizing the fermentation duration in one tank

Optimizing the use of tanks and predicting their availability during the fermentation period (1 to 2 months) is of great practical interest. We studied how to decrease the total amount of cooling power and we clarified the impact of power limitation on the fermentation duration. We proved that the temperature profile which minimizes the global amount of cooling power for one tank is the one which also minimizes the fermentation duration. The minimization is achieved not only through cooling energy, but also through nitrogen addition. Only one addition is possible, at two different times: at the beginning of the fermentation or at middle fermentation (stationary phase). The amount of added nitrogen is upper bounded, so is the available cooling power.

Minimum time problems are very common in optimization problems. This is no longer true when state-variable inequality constraints have to be taken into account. The numerical solving of such an optimal problem is generally not an easy task. The difficulty is reinforced by the constraint related to nitrogen addition.

Optimizing the fermentation duration in one tank actually consists in optimizing a temperature profile. We give below first the optimal solutions with nitrogen addition and without it, and then the practical solutions that we implemented.

Optimal solution without nitrogen addition. During the fermentation, we have two cases.

a) In the first case, the maximal cooling power is sufficiently large to accommodate all needs. The optimal solution has then 3 phases:

Phase 1: The cooling power is off from the beginning of the fermentation until the time when the temperature reaches T_{max}.

Phase 2: The cooling power is such that the temperature remains lower than T_{max}.

Phase 3: The cooling power is off when the power supplied by the fermentation is less than the power dissipated in the winery.

b) The second case arises when the maximal cooling power is a limiting factor. Then a free evolution of the temperature to its maximum (with cooling power off) would make the fermentation reach a point where the power supplied by the fermentation is greater than the maximal available cooling power. Therefore it would not be possible to keep the temperature lower than T_{max}. So, in this second case, the optimal solution described previously has to be modified as follows: during the phase 1, the cooling power is used (at its maximal value) sufficiently soon (this moment has to be determined optimally) to ensure that when the temperature of the tank reaches T_{max}, the power available for cooling is greater than the power supplied by the fermentation. Phases 2 and 3 remain unchanged.

Optimal solution with nitrogen addition. Following the solution described in the previous paragraph, and under the restriction that only one nitrogen addition is allowed, we have to consider two cases:

c) The maximal available cooling power is sufficiently large, *i.e.* the available cooling power is always greater than the power supplied by the fermentation activity with a nitrogen addition. Since the nitrogen addition (strongly) increases the fermentation activity, the optimal solution corresponds to a nitrogen addition at the beginning.

d) The maximal available power is limited. It is then necessary to add the nitrogen during the stationnary phase of the fermentation, when the fermentation activity after nitrogen addition is lower. By doing so, the available cooling power is sufficient to cool the tank.

Practical solution for all cases above:

Following that, a numerical algorithm was developed [1]. The main idea is to approximate the optimal temperature profile by a linear piecewise curve, where the slopes and the points of discontinuity of this curve match the parameters which have to be optimized. Increasing the number of parameters which describe the approximated temperature profiles allows to improve the quality of the approximation, but also intensifies the computation burden. The qualitative properties of the optimal temperature profile can *a priori* provide a parameterization of the temperature curve which proves to be efficient, even with a low number of parameters.

2.2 Decision support for the whole winery

Winery management involves a complex optimization problem, with a practical need for compromise between tank availability and energy savings while maintaining good fermentation conditions.

Fuzzy logic is therefore used to reduce the search space by providing a fast estimate of fermentation duration.

Its capability as a powerful non-linear interpolation tool [4] allows a realistic estimate of the duration of fermentations in real time. This estimate is good enough to select the best candidates for the next step, and avoids running the time consuming mathematical models in this selection step.

The fuzzy partitions and fuzzy rules used for estimation are based on expert knowledge, making them easy to understand and to adapt. The fuzzy systems are implemented through the use of the open source portable software FisPro (http://www.inra.fr/bia/M/fispro).

Once the search space limited, heuristic approaches are applied to propose improvements on winery management, either increasing tank availability by modifying fermentation control conditions or reducing power peaks by shifting the start times of fermentations.

2.3.1 Increasing tank availability

New temperature profiles and nitrogen additions are proposed to increase tank availability.

The following constraints are respected in the search process: initial and final requested temperatures, and a maximum fermentation duration, if specified.

The algorithm includes two steps.

First step: to estimate the duration of fermentation in basic configurations

In basic configurations, no nitrogen is added, and temperature is allowed to vary freely within the specified range. The fuzzy partitions and the three fuzzy rule-based systems are given in [6].

The fuzzy systems run in a very short time (less than 1 ms for 100 tanks on a regular PC) and give an estimated fermentation time with a maximum error of 5%.

Second step: trying to increase tank availability

Given a fermentation duration constraint, the addition of nitrogen and/or the choice of freely changing temperature profiles are examined and the best solution is retained. Simulations are then run to replace the

estimated times with model-based values. The overall running time for the algorithm is only a few seconds for 100 tanks on a medium-range PC.

The user can also define a compromise between tank availability and power peaks.

2.3.2 Reducing power peaks by shifting fermentation start times

When solving the system of differential equations (1), cumulative power requirements are calculated at each time, t, over the fermentation periods for all tanks. Peaks are identified by considering the highest values for cumulative power requirements.

There are usually several peaks, with several tanks contributing to each peak. An iterative algorithm identifies the tanks contributing most to the power peaks. The fermentation start times of these tanks are then shifted by one or two days, which is reasonable considering the practical constraints in wineries. The only required computation concerns cumulative power requirements, which must be calculated for each combination. The best configuration is retained and the process is repeated. This algorithm is shown schematically in figure1.

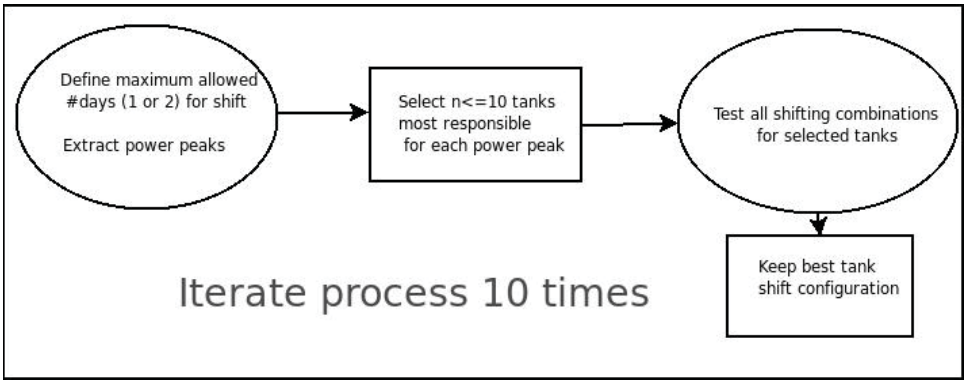

Figure 1. Heuristic approach for reducing power peaks.

3 Results

The mathematical models and optimization methods described above have been implemented in an integrated simulation software called *Sofa*, which stands for *Simulation and Optimization of Alcoholic Fermentation in winemaking conditions*. The challenge was to provide the software with the ability to simultaneously handle enough fermentations to be usable in practice for a winemaker in charge of a cellar.

The simulation engine is written in C++ and manages up to a hundred different tanks, with a response time of a few seconds and a user-friendly interface.

In our opinion, Sofa is a good example of complementarities between artificial intelligence tools and a mathematical model based simulator.

3.2 Simulation

Many situations of practical interest may be simulated by changing (i) the characteristics of the must (sugar and assimilable nitrogen concentrations) and (ii) the way in which temperature and nitrogen are managed. The simulation software is particularly useful for such studies as it provides a tool for quantification and visualization. An example is given below, about temperature management.

Temperature has a major effect on the duration of the fermentation and the maximum rate of sugar consumption, which doubles if the temperature is increased by about 8°C. The advantages of increasing the temperature during fermentation, particularly for white wines, are shown in Figure 2. Increasing the temperature from 15 to 22 °C during the second half of the fermentation radically changes the kinetics, with sugar consumption rate increasing slightly during the increase in temperature. The total duration of the fermentation is 33% shorter than the one for a fermentation carried out entirely at 15°C (duration of the second half of the fermentation 53% shorter). The maximum rate of sugar consumption is 33% lower than that for a fermentation run at 22°C. The power peak required for temperature regulation and the loss of volatile compounds are also lower.

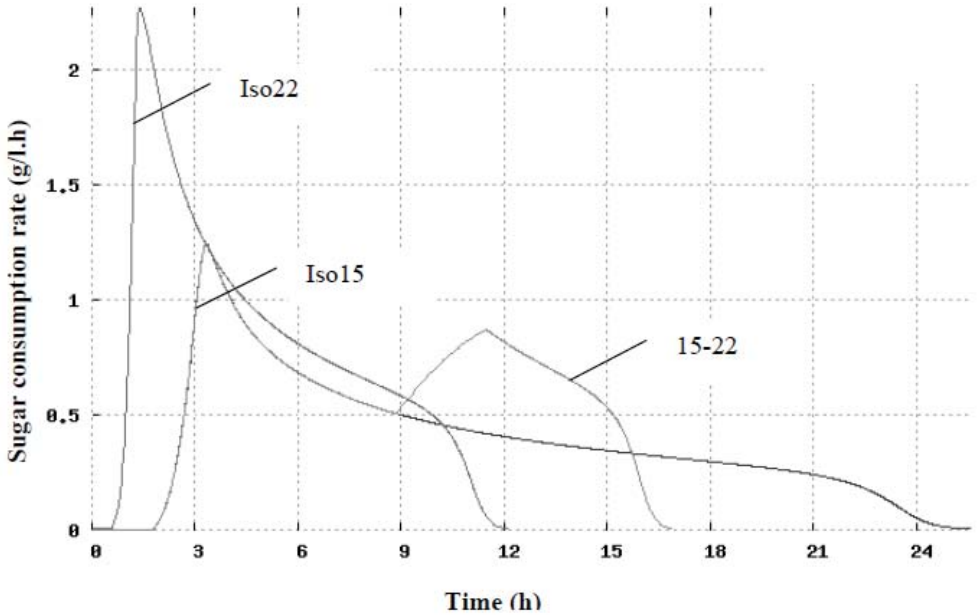

Figure 2. Simulation of the effect of temperature profile on changes in sugar consumption rate. Comparison of two isothermal fermentations (at 15 and 22°C) and an anisothermal fermentation (initial temperature = 15°C, increase to 22°C at the midpoint of fermentation)

3.2 Decision support

The decision support module calculates an "optimal" solution, by combining simulation and fuzzy logic approaches. The solutions proposed may be very useful for assessing the potential value of changes to fermentation management. Winemakers may try to increase tank availability, making it possible to ferment all the available musts. Reducing power peaks for the temperature regulation of all tanks within a winery may also be an important objective, particularly if the refrigeration unit is not very large. To do that, the decision support module calculates the potential reduction of power peaks by shifting fermentation start times.

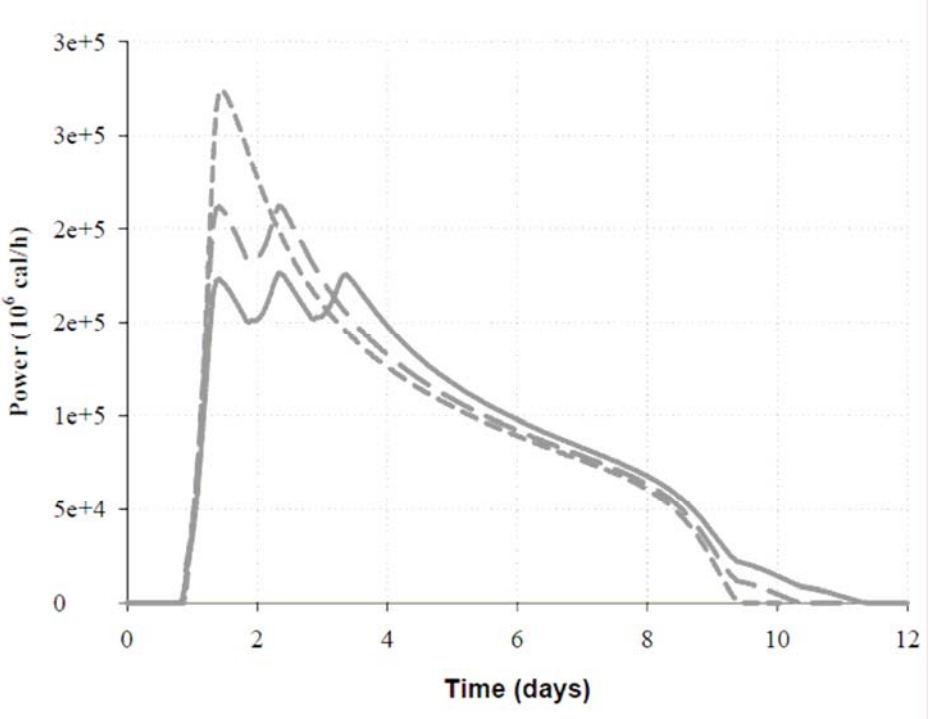

Figure 3. Application of the decision support module to reduction of the power peak. Short dashes: Initial change in power required to regulate the temperature of 100 tanks; long dashes: start time shifted by one day, solid line: start time shifted by two days.

An example of power peak reduction is shown schematically in figure 3, with 100 tanks containing the same must and regulated in the same conditions (constant temperature). This figure shows the changes in power required to regulate all the tanks when fermentations are started at the same time and the power curves after

optimization by shifting the fermentation start times of some tanks by 1 or 2 days. In those conditions, the maximum peaks are decreased by 23 % and 36%, respectively.

Conclusion

Alcoholic fermentations may be simulated by combining kinetic and thermal models. Using a decision support module, it is possible to propose better solutions for tank management and power optimization. The use of fuzzy logic makes it possible to provide elegant and efficient solutions for a complex optimization problem, using a heuristic approach based on interpretable rules.

This application is of practical value in that it can help to improve the understanding and control of fermentations and a commercial version is available (*). It could become even more useful in the future if these functions were combined with kinetic monitoring online. The corresponding control software would be able to run predictive and optimized control. In the long term, other improvements could be made, such as (i) the inclusion of quality markers (e.g. fermentation by-products) in both automatic monitoring and the models and (ii) more sophisticated decision support modules, with the possibility of changing parameters other than temperature profile and the addition of ammoniacal nitrogen.

(*) SOFA® software, INRA-Intelli'oeno.

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