# OPTIMAL CONTROL OF A FERMENTATION PROCESS

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**Keywords:** nonlinear systems, batch fermentation processes, optimal control, beer fermentation.

## Abstract

This paper includes the description of a batch beer fermentation process that has been optimised using a technique based on the application of calculus of variations. The gradient method in function space is thus introduced as a valuable tool for the optimal control of the beer fermentation process selected. The results obtained for three different cases using this method are also included.

## 1 Introduction

The term "fermentation" is derived from the Latin verb fervere, that means to boil, thus describing the appearance of the action of yeast on extracts of fruit or malted grain [9]. Yeast is a single-celled micro organism that reproduces by maturing. The conventional way for beer fermentation is to add yeast to the worth and wait for some time, letting the yeast consume substrates and produce ethanol (without stirring). According to the industry, lager yeast strains are best used at temperatures ranging from 7 to 15ºC [5]. Herewith, lager yeasts develop slower than ale yeasts, and with less surface foam they tend to settle down to the bottom of the fermentor close to the end of the fermentation (referred to as bottom yeasts). The ultimate flavour of the beer depends significantly on the strain of lager yeast and the temperatures at which it was fermented. Thus, fermentation can be accelerated with an increase of temperature but, however, some contamination risks (Lactobacillus, etc.) and undesirable by-products (diacetyl, ethyl acetate, etc.) could appear.

Biotechnological processes, as the fermentation one, may be conveniently classified according to the mode chosen for process operation: either batch, fed-batch or continuous [6]. During batch operation of a process, no substrate is added to the initial charge nor is product removed until the end of the process. Conditions are continuously changing with time, and the fermentor is an unsteady-state system, although in a well-mixed reactor, conditions can be assumed to be consistent throughout the reactor at any instant of time [4].

Most real life processes cannot be represented by a deterministic model (an exact representation of the process) because of the dynamic nature of the process and the lack of information and other uncertainties being associated with the available data. In practice, all systems are usually non-linear and, therefore, may exhibit forms of behaviour that are not at all apparent from the study of the linearised versions. The model is not expected to be a reconstruction of the process, rather it is intended to serve as a set of operators on the identified set of inputs, producing similar output as expected from the process.

Continuous constrained optimisation techniques such as bound-constrained optimisation problems, play an important role in the development of software for the general constrained problem because many constrained codes reduce the solution of the general problem to the solution of a sequence of bound-constrained problems. It is also important in applications because parameters that describe physical quantities are often constrained to lie in a given range [3].

A method of first order gradients is probably the easiest and most stable computation of optimal control, because if the system state equations are stable in forward time then the co-state equations are stable when integrated in reverse time. Convergence is not usually critically dependent on a first approximation. For the particular case of the continuous process that the beer fermentation presents, a direct method known as the gradient method in function space has been selected [2, 8].

## 2 The Batch Beer Fermentation Process

The mathematical model chosen to be part of the simulation (and subsequently the optimisation process) is the kinetic model by Andres-Toro et al. [1] since it has been obtained from many experimental studies at laboratory scale showing good results. It takes into account realistic aspects of the process such as characteristics of the wort and yeast, and also two important by-products of the fermentation: ethyl acetate and diacetyl.

Biomass is segregated into three different types of cells: lag, active and dead. The whole process can be divided in two successive phases: a lag phase and a fermentation phase. A scheme of the process with its main variables is presented in Figure 1. Table 1 describes the nomenclature used for this mathematical model.

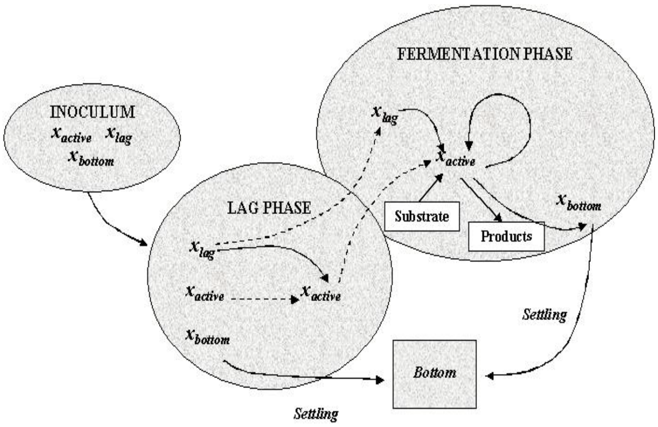

Fig. 1: Process scheme for the kinetic model [1].

| Parameter | Description | Unit |
|---|---|---|
| $\mu_a$ | Ethanol production rate | $h^{-1}$ |
| $\mu_D$ | Specific yeast settling down rate | g/l |
| $\mu_{eas}$ | Ethyl acetate coefficient rate | g/l |
| $\mu_{lag}$ | Specific rate of latent formation | $h^{-1}$ |
| $\mu_s$ | Substrate consumption rate | $h^{-1}$ |
| $\mu_x$ | Specific yeast growth rate | $h^{-1}$ |
| *acet* | Ethyl acetate concentration | ppm |
| *diac* | Diacetyl concentration | ppm |
| *e* | Ethanol concentration | g/l |
| *f* | Fermentation inhibitor factor | g/l |
| $k_{dc}$ | Diacetyl appearance rate | |
| $k_{dm}$ | Diacetyl reduction rate | |
| $k_m$ | Yeast growth inhibition parameter | g/l |
| $k_s$ | Sugar inhibition parameter | g/l |
| *s* | Concentration of sugar | g/l |
| $s_0$ | Initial concentration of sugar | g/l |
| *t* | Time | h |
| *T* | Temperature | °C |
| $x_{active}$ | Suspended active biomass | g/l |
| $x_{dead}$ | Suspended dead biomass | g/l |
| $x_{lag}$ | Suspended latent biomass | g/l |

Table 1: Nomenclature used

Herewith, the enunciation of the model corresponding to the lag and fermentation phases is as follows:

$$\frac{dx_{lag}}{dt} = -\mu_{lag} \cdot x_{lag} \tag{1}$$

$$\frac{dx_{active}}{dt} = \mu_x \cdot x_{active} - k_m \cdot x_{active} + \mu_{lag} \cdot x_{lag} \tag{2}$$

$$\frac{dx_{dead}}{dt} = k_m \cdot x_{active} - \mu_D \cdot x_{dead} \tag{3}$$

$$\frac{ds}{dt} = -\mu_s \cdot x_{active} \tag{4}$$

$$\frac{de}{dt} = \mu_a \cdot f \cdot x_{active} \tag{5}$$

To describe the evolution of the by-products that have an important impact (ethyl acetate contributes with a fruity odour and flavour, and diacetyl makes beer heavy and sweet flavoured), the following equations are established:

$$\frac{d(acet)}{dt} = \mu_{eas} \cdot \mu_s \cdot x_{active} \tag{6}$$

$$\frac{d(diac)}{dt} = k_{dc} \cdot s \cdot x_{active} - k_{dm} \cdot diac \cdot e \tag{7}$$

The remaining parameter equations can be calculated as follows:

$$x_{total} = x_{active} + x_{lag} + x_{dead} \tag{8}$$

$$\mu_x = \frac{\mu_{x0} \cdot s}{0.5 \cdot s_0 + e} \tag{9}$$

$$\mu_D = \frac{0.5 \cdot s_0 \cdot \mu_{D0}}{0.5 \cdot s_0 + e} \tag{10}$$

$$\mu_s = \frac{\mu_{s0} \cdot s}{k_s + s} \tag{11}$$

$$\mu_a = \frac{\mu_{a0} \cdot s}{k_s + s} \tag{12}$$

$$f = 1 - \frac{e}{0.5 \cdot s_0} \tag{13}$$

Since the process depends on temperature, the value of all parameters of the model is calculated by exponential equations of the Arrhenius type ($\mu = A \cdot e^{\frac{B}{RT}}$). The constant values of $k_{dc}$ and $k_{dm}$ were calculated with the experimental data for the diacetyl concentration's behaviour:

$$\mu_{x0} = 1.095 \times 10^{47} \cdot e^{\frac{-63720}{1.99536 \cdot (T+273.15)}} \tag{14}$$

$$k_m = 3.373 \times 10^{56} \cdot e^{\frac{-76450}{1.99536 \cdot (T+273.15)}} \tag{15}$$

$$\mu_{eas} = 1.129 \times 10^{39} \cdot e^{\frac{-53056}{1.99536 \cdot (T+273.15)}} \tag{16}$$

$$\mu_{D0} = 4.889 \times 10^{14} \cdot e^{\frac{-20020}{1.99536 \cdot (T+273.15)}} \tag{17}$$

$$\mu_{s0} = 6.232 \times 10^{-19} \cdot e^{\frac{23254}{1.99536 \cdot (T+273.15)}} \tag{18}$$

$$\mu_{a0} = 26.3865 \cdot e^{\frac{-2528.6}{1.99536 \cdot (T+273.15)}} \tag{19}$$

$$\mu_{lag} = 2.2041 \times 10^{13} \cdot e^{\frac{-18959}{1.99536 \cdot (T+273.15)}} \tag{20}$$

$$k_s = 1.1081 \times 10^{-52} \cdot e^{\frac{68249.2}{1.99536 \cdot (T+273.15)}} \tag{21}$$

$$k_{dc} = 0.000127672 \tag{22}$$

$$k_{dm} = 0.00113864 \tag{23}$$

## 3 Formulation of The Optimal Control Problem

The beer fermentation model described in Section 2 has been implemented in the SIMULINK environment. This implemented model includes the objective function to be maximised. The original objective function defined intends to reach the required ethanol level in the industrial fermentation without quality loss or contamination risks and also maintaining a good implementable profile for the industry [1]. The following sub functions are defined including penalty parameters to obtain an approximation of an objective function to be maximised:

$$J_1 = 10 \cdot e(t_f) \tag{24}$$

$$J_2 = -5.73 \times 10^{-8} \cdot e^{(95 \cdot diac(t_f))} \tag{25}$$

$$J_3 = -1.16 \times 10^{-29} \cdot e^{(4.6 \cdot acet(t_f))} \tag{26}$$

$$J_4 = -\int_0^{t_f} 9.91 \times 10^{-17} \cdot e^{(2.31T)} dt \tag{27}$$

$$J_5 = -\sum_{i=1}^{N} \frac{|T_{i+1} - T_i|}{\Delta t} \tag{28}$$

with $N\Delta t = t_f$.

The intention of each of these factors in the objective function is as follows: $J_1$ measures the final ethanol production, $J_2$ limits the level of ethyl acetate at the end, $J_3$ limits the diacetyl concentration at the end, $J_4$ limits the temperature along the process, and $J_5$ penalises brisk changes in temperature.

These terms together provide an overall cost function of the process:

$$J = J_1 + J_2 + J_3 + J_4 + J_5 \tag{29}$$

Following the simulation of the industrial profile and after several experimentation with the SIMULINK model of the process [2]; the terms $J_2$ and $J_3$ have been found to be negligible compared with $J_1$. The last term $J_5$ has been ignored at this stage in order to simplify the optimal control formulation and as a result, there is a significant reduction to the objective function and number of state equations. These conditions can be considered a special case for the optimisation where $J_2 = J_3 = J_5 = 0$.

With this, a new performance index $J_r$ can be described as follows:

minimise

$$J_r = -10e(t_f) + \int_0^{t_f} 9.91 \times 10^{-17} \cdot e^{(2.31T)} dt \tag{30}$$

subject to

$$\frac{dx_{lag}}{dt} = -\mu_{lag}(T) x_{lag} \tag{31}$$

$$\frac{dx_{active}}{dt} = \frac{\mu_{x0}(T)s}{0.5s_0 + e} x_{active} - k_m(T) x_{active} + \mu_{lag}(T) x_{lag} \tag{32}$$

$$\frac{ds}{dt} = -\frac{\mu_{s0}(T)s}{k_s(T) + s} x_{active} \tag{33}$$

$$\frac{de}{dt} = \frac{\mu_{a0}(T)s}{k_s(T) + s}\left(1 - \frac{e}{0.5s_0}\right) x_{active} \tag{34}$$

Together with this, the reduced state and control signals ($x_i$ and $u$) are defined:

$$x_1 = x_{lag},\ x_2 = x_{active},\ x_3 = s,\ x_4 = e,\ u = T$$

Subsequently, replacing these variables in equations 30-34 for the special case:

$$J_r = -10x_4(t_f) + \int_0^{t_f} ce^{du} dt \tag{35}$$

$$\frac{dx_1}{dt} = -\mu_{lag}(u)x_1,\ \ x_1(0) = 2 \tag{36}$$

$$\frac{dx_2}{dt} = \frac{\mu_{x0}(u)x_3}{0.5s_0 + x_4} x_2 - k_m(u)x_2 + \mu_{lag}(u)x_1,\ \ x_2(0) = 0.5 \tag{37}$$

$$\frac{dx_3}{dt} = -\frac{\mu_{s0}(u)x_3}{k_s(u) + x_3} x_2,\ \ x_3(0) = 130 \tag{38}$$

$$\frac{dx_4}{dt} = \frac{\mu_{a0}(u)x_3}{k_s(u) + x_3}\left(1 - \frac{x_4}{0.5s_0}\right) x_2,\ \ x_4(0) = 0 \tag{39}$$

where the given initial conditions are stated and:

$$\mu_{lag}(u) = 2.2041 \times 10^{13} e^{\frac{-18959}{R(u+T_a)}} \tag{40}$$

$$\mu_{x0}(u) = 1.095 \times 10^{47} e^{\frac{-63720}{R(u+T_a)}} \tag{41}$$

$$\mu_{s0}(u) = 6.232 \times 10^{-19} e^{\frac{23254}{R(u+T_a)}} \tag{42}$$

$$\mu_{a0}(u) = 26.3865 e^{\frac{-2528.6}{R(u+T_a)}} \tag{43}$$

$$k_m(u) = 3.373 \times 10^{56} e^{\frac{-76450}{R(u+T_a)}} \tag{44}$$

$$k_s(u) = 1.1081 \times 10^{-52} e^{\frac{68249.2}{R(u+T_a)}} \tag{45}$$

with $R = 1.99536$; $T_a = 273.15$; $c = 9.91 \times 10^{-17}$ and $d = 2.31$.

The optimisation problem can thus be written in the form:

minimise

$$J_r = \Phi\left(x(t_f)\right) + \int_0^{t_f} ce^{du} dt \tag{46}$$

subject to

$$\dot{x} = f(x,u),\ x(0) = x_o \tag{47}$$

where

$$f(x,u)=\begin{bmatrix} -\mu_{lag}(u)x_1 \\ \left(\frac{\mu_{x0}(u)x_3}{0.5s_0+x_4}-k_m(u)\right)x_2+\mu_{lag}(u)x_1 \\ -\frac{\mu_{s0}(u)x_3}{k_s(u)+x_3}x_2 \\ \frac{\mu_{a0}(u)x_3}{k_s(u)+x_3}\left(1-\frac{x_4}{0.5s_0}\right)x_2 \end{bmatrix} \qquad (48)$$

$$x(0)=\begin{bmatrix} 2 \\ 0.5 \\ 130 \\ 0 \end{bmatrix}$$

$$\Phi\left(x(t_f)\right)=-10x_4(t_f)$$

## 4 Application of Calculus of Variations

The standard necessary optimality conditions for an unconstrained optimal control problem can be found by means of *calculus of variations*. This principle is now applied to the optimisation problem and thus, the Hamiltonian (*H*) can be defined as [7]:

$$H=ce^{du}+p^T f(x,u) \qquad (49)$$

Therefore, the Hamiltonian gradient can be represented as follows:

$$H_u=\frac{dH}{du}=cde^{du}+\left[\frac{\partial f}{\partial u}\right]^T p \qquad (50)$$

One of the necessary optimality conditions for a local maximiser is that this gradient should be equal to zero, so that:

$$u=\frac{\log_e\left(-\frac{\left[\frac{\partial f}{\partial u}\right]^T p}{cd}\right)}{d} \qquad (51)$$

It is important to note that since *c* and *d* are both positive, the equation 51 will only give a valid (real) result for *u* when:

$$\left[\frac{\partial f}{\partial u}\right]^T p<0 \qquad (52)$$

The co-state equations are:

$$\dot{p}=-\nabla_x H,\ p(t_f)=\left.\frac{\partial\Phi}{\partial x}\right|_{x=x(t_f)} \qquad (53)$$

which gives as a result:

$$\dot{p}=-\left[\frac{\partial f}{\partial x}\right]^T p,\ p(t_f)=\begin{bmatrix}0 & 0 & 0 & -10\end{bmatrix}^T \qquad (54)$$

where $\left[\frac{\partial f}{\partial x}\right]$ and $\left[\frac{\partial f}{\partial u}\right]$ are the Jacobian matrices given by:

$$A(x,u)=\left[\frac{\partial f}{\partial x}\right]=\begin{bmatrix} a_{1,1}(u) & 0 & 0 & 0 \\ a_{2,1}(u) & a_{2,2}(x,u) & a_{2,3}(x,u) & a_{2,4}(x,u) \\ 0 & a_{3,2}(x,u) & a_{3,3}(x,u) & 0 \\ 0 & a_{4,2}(x,u) & a_{4,3}(x,u) & a_{4,4}(x,u) \end{bmatrix}$$

$$B(x,u)=\left[\frac{\partial f}{\partial u}\right]=\begin{bmatrix} b_1(x,u) \\ b_2(x,u) \\ b_3(x,u) \\ b_4(x,u) \end{bmatrix}$$

Then, the value of the different terms of these matrices can be calculated with partial derivatives from equations 36-39 and the initial conditions.

## 5 The Gradient Method in Function Space

In order to find the numerical computation of optimal control of both continuous and discrete-time systems there are mainly two approaches according to Noton [8]: indirect and direct methods of minimisation of a performance index (objective function). In the direct approaches to minimisation, the state equations are influenced only by the control *u*(*t*) and the minimisation of the objective function *J*(*u*) by direct adjustment of *u*(*t*) is sought.

A method of first order gradients is the simplest approach to a direct method in which the state and co-state equations remain separated. The logical and convenient approach is to regard continuous time systems as the limiting case of discrete systems as the subinterval of time tends to zero.

The method of steepest descent (first order gradients) consists therefore of applying the iterative correction:

$$\Delta u(t)=-e\frac{\partial H}{\partial u(t)}=-eH_u \qquad (55)$$

where *e* is an arbitrary constant provided to regulate convergence (stability). Since *H* depends on the co-state variables, the *f*(*t*) have to be generated by an iterative process.

Thus, the algorithm can be described as follows:

**Data**: $t_f$, *e*

**Step 0**: *initialisation*: Set iteration counter *k* = 1, and guess $u(t)^0$ for the interval $[0,t_f]$.

**Step 1**: Compute *x*(*t*) and $J_r$ from equations 47 and 46.

**Step 2**: Compute the co-state vector *p*(*t*) by solving equation 54 in reverse time.

**Step 3**: Compute the Hamiltonian gradient $H_u$ from equation 50.

**Step 4**: Update *u*(*t*) using equation 55. That is:

$$u(t)^{k+1}=u(t)^k-eH_u \qquad (56)$$

Set *k* = *k*+1 and repeat from **Step 1** until convergence is achieved.

Note that because equation 51 is not solved explicitly, the associated validity condition is not an issue.

Herewith, three cases have been considered in order to initialise the input temperature profile:

Case 1: $u(t)$ has been initialised at the optimal constant solution obtained using the MATLAB routine *fminbnd*, based on golden section search and parabolic interpolation, that is:

$$u(t) = 14.6211,\ t \in [0,160]$$

Case 2: $u(t)$ has been initialised at an arbitrary steady-state solution, that is:

$$u(t) = 10,\ t \in [0,160]$$

Case 3: $u(t)$ has been initialised at the industrial profile (defined by Andres-Toro et al, [1]).

For each of these cases $e = 1$ was set initially. Adaptation of this parameter was required during the optimisation routine by means of two regulating parameters $k_1$ and $k_2$ (set a priori to 1.1 and 0.75 respectively) which regulate at every iteration, the value of $e$ by multiplying either $k_1$ to increase or $k_2$ to decrease it. This adjusting procedure depends on the convergence of the real performance value obtained for every iteration.

The MATLAB routine *ode23* (low order method) was used to solve the state and co-state differential equations. The iterations were considered to have converged when an increase in the value of $J_r$ was observed. The SIMULINK model was finally used to investigate the final individual performance components. The results are summarised in Table 2.

| Case | *J(initial)* | Iter-ations | $J_r$ | *J(final)* | Total time* |
|---|---|---|---|---|---|
| 1 | 597.8082 | 48 | 601.8149 | 599.01 | 39.166 |
| 2 | 470.3171 | 253 | 601.9525 | 595.34 | 276.267 |
| 3 | 548.2027 | 273 | 601.9667 | 593.13 | 278.761 |

*Time in seconds using an 800MHz CPU PC with 256MB RAM.

Table 2: Results obtained with the gradient method

## 6 Analysis of Results

With the optimum steady-state control profile obtained, an increment in the performance index from the original 518.90 with the industry's temperature profile has been reached to a new 597.80 value. This means a percentage increase of more than 15% by making the problem formulation simpler.

With the help of an adaptation technique for the value of $e$, the optimisation results using the gradient method in function space have been satisfactory after several tests. It is significant to mention that little computational effort (overall process time) has been required to obtain the results. The value of the performance index obtained for all three cases studied has been greater than the original value with the initial profile. An important increase has been attained for Case 1, using the optimal constant profile as the initial profile (599.01). Convergence problems were reasonably few, given that to obtain the optimised solutions testing was not extensive.

The results for the maximum value of the performance index obtained among the different techniques and cases reviewed, have been included below (Case 1 using the gradient method).

Figure 2 includes a comparison between the initial and final temperature control profiles applied to the mathematical model. Then, Figure 3 shows the convergence development of the parameters $u(t)$ and $J_r$ versus the number of iterations.

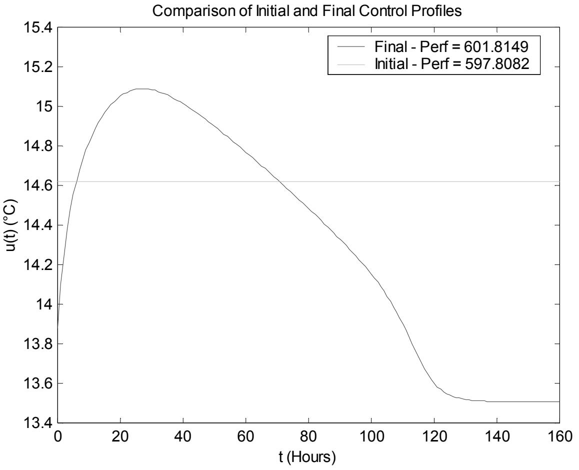

Fig. 2: Initial and final temperature profiles

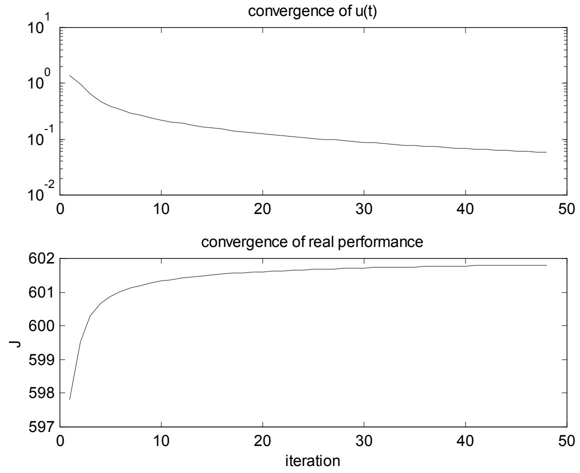

Fig. 3: Convergence of the parameters $u(t)$ and $J$

The optimised temperature profile obtained can now be applied to the SIMULINK model that includes all the variables from the original objective function. The new value of the performance index can be attained in this way. Figure 4 illustrates the SIMULINK model that includes the mathematical equations of the fermentation process, it also includes the values obtained for the different parameters using the selected Case 1 with the gradient method.

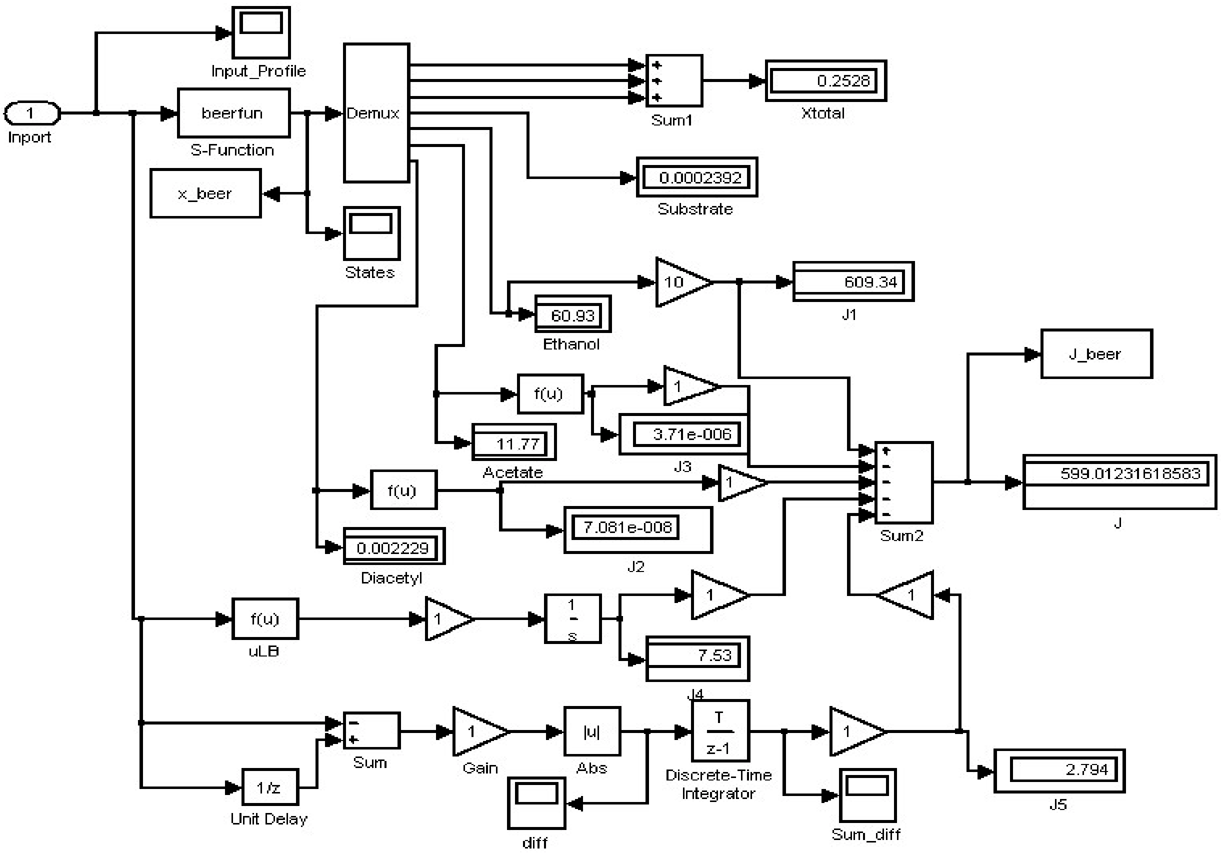

Fig. 4: SIMULINK model used for beer fermentation process

## 7 Conclusions and Further Work

In this paper, the mathematical model of a beer fermentation process has been reviewed in order to use it as the subject of optimal control. After the application of calculus of variations to the optimisation problem, a solution using a gradient method in function space has been achieved. Results for three particular cases has been included and the values achieved demonstrate how helpful this optimisation technique is for the fermentation process considered.

Further work can involve the use of different well-established optimisation methods adapted for the optimal control of the particular fermentation process included in this work.

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