OPTIMAL HEATING POLICIES FOR SURFACE DECONTAMINATION OF FRUITS

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Abstract: Here we address the problem of finding optimal heating policies for surface decontamination of fruits, considering strawberries as a case study. Hot water dips are effective for fungal pathogen control, because fungal spores are either at the surface or just beneath. However, the application of severe heating profiles can damage the fruit. We consider the optimal control problem which leads to optimal heating policies. The results show interesting, non-obvious, cyclic heating profiles.

Keywords: surface decontamination (pasteurization), optimal control, dynamic optimization, strawberries

INTRODUCTION

The food industry is under great pressure to increase efficiency, quality, safety, and minimize environmental impact. Many of its operations are performed in batch or semi-continuous mode, so they are intrinsically dynamic. The mathematical models of food processing operations have certain characteristics which will pose special difficulties for their mathematical optimisation [1]:

- Non-linear, dynamic models with possible discrete events
- Many variables of interest (temperature, concentration, etc.) are usually distributed in space, thus these models are, partially or fully, distributed systems (i.e. described by partial differential equations) usually with coupled transport phenomena
- Presence of nonlinear constraints related to safety and quality demands

Thus, these mathematical models usually consist of sets of algebraic, partial and ordinary differential equations (PDAEs), with possible integral equations, and sometimes even logic conditions (modelling discrete events and/or transitions, i.e. hybrid systems). These PDAEs models are usually transformed into DAEs via suitable spatial discretization methods (e.g. finite differences, method of lines, finite elements, etc.). In the context of process engineering, the numerical solution of NLP-DAEs is usually a very challenging task due to the highly non-linear and frequently discontinuous nature of the dynamics of most processes. In fact, these characteristics make the NLP multimodal, i.e. there is not a unique global solution. Instead, a number of local solutions are possible, so the problem becomes much more complicated since the absolute best (global) solution must be found in a reliable and efficient way. In fact, standard gradient-based techniques for NLPs (e.g. SQP) are of local nature, i.e. they will converge to one of the local solutions, and in fact without giving any information about its local nature.

In this contribution, we address the problem of finding optimal heating policies for surface decontamination of fruits, considering strawberries as a particular case study. Hot water dips are effective for fungal pathogen control, because fungal spores and latent infections are either at the surface or just beneath. However, the application of severe heating profiles can damage the fruit (strawberry in this case), causing an atypical pigmentaion plus significant loss of fruit firmness. In order to reduce the intensity of the thermal treatment while ensuring the desired microbial inactivation...
properties, cyclic variations of the water temperature can be applied. In the following, we consider the formulation and the solution of the optimal control problem which leads to optimal heating policies.

**OPTIMIZATION OF DYNAMIC SYSTEMS**

The objective of dynamic optimization (or open loop optimal control) is to find a set of control variables (which are functions of time) in order to maximize the performance of a given dynamic system, as measured by some functional, and all this subject to a set of path constraints. In general, optimal control problems can be ultimately formulated (e.g. via control parameterization) as non-linear programming (NLP) problems subject to the dynamics of the system (acting as equality constraints) and possibly to other inequality constraints. In the context of food processing, the numerical solution of these problems is usually a very challenging task due to the highly non-linear and frequently discontinuous nature of the dynamics of most processes. In fact, these characteristics make the NLP multimodal, i.e. there is not a unique global solution [1]. The mathematical formulation involves to find the control vector \( (u(t)) \), to minimize (or maximize) a performance index (functional) \( J[x,u] \):

\[
J[x,u] = \Theta[x(tf)] + \int_{0}^{t_f} \Phi[x(t),u(t),t]dt
\]

subject to

\[
\frac{dx}{dt} = \Psi[x(t),u(t),t]
\]

where equation (2) represents a set of ordinary differential equality constraints, \( x \) is the vector of state variables with initial condition \( x(t_0) = x_0 \) and also subject to sets of algebraic equality and inequality constraints such as:

\[
\begin{align*}
    h[x(t),u(t)] &= 0 \\
g[x(t),u(t)] &\leq 0
\end{align*}
\]

Furthermore, equation (4) represents the upper and lower bounds on the state and control variables,

\[
\begin{align*}
x^L &\leq x(t) \leq x^U \\
u^L &\leq u(t) \leq u^U
\end{align*}
\]

If the process is modeled as a distributed system, i.e. the state variables are function of both time and spatial position, the corresponding governing equations are introduced as an additional set of equality constraints, that is:

\[
\begin{align*}
p(x,x_k,x_{kk},...,k) &= 0 & k \in \Omega \\
q(x,x_k,x_{kk},...,k) &= 0 & k \in \delta\Omega
\end{align*}
\]

where \( k \) are the independent variables (time and spatial position). Basically, optimal control problems are solved using numerical methods that could be classified under indirect and direct approaches.

**GLOBAL OPTIMIZATION METHODS**

In this study, we have considered an indirect approach based on control vector parameterization (CVP) scheme [1]. Since the resulting NLPs are usually non-convex, we have considered a set of selected global optimization (GO) methods which can handle black-box models. The selection has been made based on their published performance and on our own experiences [1]. Although none of these methods can guarantee optimality, they locate the vicinity of global solutions (often the best available) with relative efficiency. The GO methods which we have considered are:
**ICRS:** an stochastic GO method presented by Banga and Casares [2], improving the Controlled Random Search (CRS) method of Goulcher and Casares [3]. Basically, ICRS is a sequential (one trial vector at a time), adaptive random search method which can handle inequality constraints via penalty functions.

**DE:** the Differential Evolution method [4] is a heuristic, population-based approach to GO. The original code of the DE algorithm [4] did not check if the new generated vectors were within their bound constraints, so we have slightly modified the code for that purpose.

**SRES:** the Evolution Strategy using Stochastic Ranking [5] is a $(\mu, \lambda)$-ES evolutionary optimization algorithm which uses stochastic ranking as the constraint handling technique. The stochastic ranking is based on the bubble-sort algorithm and is supported by the idea of dominance. It adjusts the balance between the objective and penalty functions automatically during the evolutionary search.

**OPTIMAL POLICIES FOR SURFACE DECONTAMINATION**

Thermal treatment is widely used as a preservation technique to extend the shelf life of food products. Fungal decay through thermal treatments is very effective because it targets a direct inactivation of pathogens. Since fungal spores and latent infections are either operating on the surface of fruit and vegetables, or just beneath, hot water dips are useful for decontamination of the product [6]. It has also been described that a thermal treatment at a high constant temperature during a time period might affect the internal structure and can lead to the malfunctioning of vital components. In case of strawberries, this effect implies loss of fruit firmness, and the development of atypical pink pigmentation of the fruit [7]. However, the application of periodic variations of the water temperature produces a superficial heating of strawberries without damaging them [8]. Empirical studies [8] also concluded that in order to keep the organoleptic properties of the fruit as well as to achieve the desired microbial inactivation, pulse profiles should be considered.

It was assumed that inside the strawberry heat is mainly transferred by means of conduction. At the boundary surface of the strawberry, denoted by $\Gamma$, it was assumed that heat is transferred by means of convection to its surrounding environment.

\[
\rho(T) \frac{c(T)}{c(T)} \frac{\partial T}{\partial t} = \nabla \left[ \lambda(T) \nabla T \right]
\]

\[
\lambda(T) \frac{\partial T}{\partial n} = h \left[ T - T_a(t) \right]
\]

\[
T(t = t_0, x, y, z) = T_0
\]

where $T$ [°C] is the temperature inside the fruit, $\rho$ is the density [kg/m³], $c$ is the heat capacity [kJ/(kg °C)], $\lambda$ is the thermal conductivity [W/(m °C)] of the strawberry, $n$ is the outward normal to the strawberry surface $\Gamma$, $h$ is the surface heat transfer coefficient [W/(m² °C)], and $T_a(t)$ is the ambient temperature [°C]. At the beginning of the thermal treatment, i.e., $t = t_0$, the temperature distribution inside the strawberry was considered to be uniform with $t_0$ the starting time [s], $T_0$ a constant temperature [°C] and $x, y, z$ Cartesian spatial coordinates [m]. In this work, the thermal properties were assumed to be temperature independent, a reasonable assumption for the temperature range considered.

In order to reduce the computational effort in each iteration step of the optimization procedures, the actual 3D shape of strawberry was estimated using a spherical geometric model. The radius of the sphere – determined by measuring the average height and diameter of 162 berries – was 19 mm. The volume was then calculated based on the average radius. The density of each strawberry was calculated and the average used for further calculations, was 803 kg/m³. The thermophysical properties were estimated based on the chemical composition of strawberries, and the inactivation properties of Botrytis cinerea were used [8].

The local change of microbial population, $N$ [cfu/ml], at the surface, $\Gamma$, of a strawberry is modeled as a first-order decay reaction:

\[
\frac{dN}{dt} = -kN
\]
During surface decontamination the microbial inactivation rate, $k \, [1/\text{min}]$, is temperature dependent and is described using an Arrhenius-type equation,

$$ k(T) = k_{\text{ref}} \exp \left[ \frac{E_a}{R} \left( \frac{1}{T_{\text{ref}} + 273} - \frac{1}{T + 273} \right) \right] $$

where $k_{\text{ref}} \, [1/\text{min}]$ is the inactivation rate at a reference temperature $T_{\text{ref}} \, [\degree \text{C}]$, $E_a$ is the inactivation energy $[\text{J/mol}]$, and $R \, [\text{J/(mol \degree \text{C})}]$ is a universal constant. The actual value of the inactivation rate, $k(T)$, is determined by the local temperature at a given point on the surface of the strawberry. Since the values of $N$ decrease exponentially with time, a change of variables is introduced to avoid numerical problems during the computation process, that is, $n(t,x,y,z)=-\log N(t,x,y,z)$. Substitution of this equation into the differential system yields

$$ \frac{dn}{dt} = \frac{k(T)}{2.3} $$

$$ n = n(t,x,y,z), \, \{x,y,z\} \in \Gamma $$

$$ n(t=t_0,x,y,z) = n_0 = -\log N_0 $$

At a given time point, $t$, during decontamination, the total microbial population at the surface of the strawberry, $m_t$, is computed as follows:

$$ m_t = \frac{\int_{\Gamma} N(t,x,y,z) \, d\Gamma}{\int_{\Gamma} \, d\Gamma} $$

The intensity of the thermal treatment, while ensuring a desired level of surface decontamination, can be reduced by applying a cyclic variation of the ambient (water) temperature. To penalise for excessive heating and to take into account its spatial and temporal distribution, the following quantitative measure is introduced as objective function to be minimized:

$$ J(t) = \int_{t_0}^{t} \left[ \exp \left[ T(t,x,y,z) - T_0(t,x,y,z) \right] \right] \, d\Omega \, dt $$

subject to

$$ T_{\text{max}} \leq 48.0 \quad (\degree \text{C}) $$

$$ M_t \geq 3.5 \quad (\log-\text{units}) $$

$$ \delta t \geq 1.0 \quad (\text{min}) $$

where the constraints $T_{\text{max}}$, $M_t$, and $\delta t$ are the maximum temperature in the domain at final time, the microbial load at final $t$ and the minimum duration of each heating cycle respectively.

**RESULTS**

Each of the GO methods considered has several adjustable search parameters which can greatly influence their performance, both in terms of efficiency and robustness. We have followed the published recommendations for each method ([9,10,11,4]), together with the feedback obtained after a few preliminary runs. All the computation times were obtained using a PC Pentium III/866 MHz. For the sake of fair comparison, we have considered Matlab implementations of all the GO methods since it is a convenient environment to postprocess and visualize all the information arising from the optimization runs of the different solvers.
The resulting NLP problem had 20 decision variables after using CVP with a piecewise constant discretization for the control. The upper and lower bounds for the decision variables were (20, 48 °C) in the case of temperature and (1, 20 min) for the duration of every time element. Finally, in order to analyse the influence of the treatment time, the optimization problem was solved for different final times of 20, 30, 40, 50 and 60 minutes respectively.

Table 1 shows the best result obtained for each treatment time. The best method was always the DE stochastic algorithm, although ICRS and SRES converged to very similar values. In order to provide a more fair comparison of the different methods, a plot of the convergence curves for the case of 60 min (objective function values versus computation time) is presented in Figure 1, where the best three curves per method from a set of 30 are plotted. The ICRS algorithm always presented an initial faster convergence to the optimum although at the end it is slightly surpassed by the DE method.

As an example, the optimal profile obtained for 60 min. is presented in Figure 2. It should be noted that the obtained optimal controls confirm the initial hypothesis about the advantages of applying pulse profiles. The profiles for the other cases are not shown here, but the behavior observed is similar to the treatment of 60 min. In order to show the improvement obtained by the pulse heating profiles, Figure 3 shows the value of the objective function for the optimal and nominal processes (only one heating step of constant temperature) for different treatment times. It should be noted that the optimal process always implies a lower objective function value than the nominal one.

Table 1: Summary of best results, obtained with DE

<table>
<thead>
<tr>
<th>Treatment time (min)</th>
<th>Objective function</th>
<th>CPU time (h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.36·10^9</td>
<td>5.89</td>
</tr>
<tr>
<td>30</td>
<td>1.28·10^9</td>
<td>6.97</td>
</tr>
<tr>
<td>40</td>
<td>9.29·10^8</td>
<td>7.98</td>
</tr>
<tr>
<td>50</td>
<td>7.55·10^8</td>
<td>7.76</td>
</tr>
<tr>
<td>60</td>
<td>6.60·10^8</td>
<td>7.94</td>
</tr>
</tbody>
</table>

Figure 1.- Convergence curves

Figure 2.- Optimal heating policies

Figure 3.- Optimal vs nominal processes

Figure 4.- Histogram of local optima (msSQP)
In order to illustrate the multimodality of this problem, it was also solved using the multi-start SQP (Sequential Quadratic Programming) approach, considering 100 random initial vectors, which were generated satisfying the decision variables bounds. SQP is considered the state of the art in local methods for NLPs. The results correspond to a large number of local solutions, as depicted in the histogram shown in Figure 4.

It is very significant that despite the huge computational effort associated with the 100 SQP runs, the best value found was still far from the solutions of several of the GO methods, obtained with much smaller computation times. These results illustrates well the inability of the multi-start approach to handle highly multimodal problems like this one.

CONCLUSIONS

Hot water dips are frequently used for the surface pasteurization of fruits. The application of severe heating profiles can damage the fruit (strawberry in the case considered here), causing an atypical pigmentation plus significant loss of fruit firmness. In order to reduce the intensity of the thermal treatment while ensuring the desired microbial inactivation properties, cyclic variations of the water temperature have been suggested as better alternatives to current practice [8].

Here we have considered the formulation and the solution of the optimal control problem which leads to optimal heating policies for surface pasteurization. Using suitable global optimization methods, we have found that optimal operating procedures are indeed cyclic and provide significant improvements over nominal processes. It was also proved that standard NLP local methods (like SQP) are not able to solve this problem adequately, even after considering a multi-start strategy. These results reinforce the importance of global optimization techniques for improving food processing [1].

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