Model predictive control of the primary drying stage of the drying of solutions in vials: an Application of the MPC@CB Software (Part 1)

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MODEL PREDICTIVE CONTROL OF THE PRIMARY DRYING STAGE OF A FREEZE DRYING OF SOLUTIONS IN VIALS: A APPLICATION OF THE MPC@CB SOFTWARE (PART 1)

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This paper deals with the first principle model based predictive control of the primary drying stage of a freeze drying of solutions in vials. In the proposed control approach, any online control problem concerned with a constrained optimization during the primary drying stage may be stated. It is solved using a special model predictive control framework where the model is used in the controller formulation. Our first simulation results show here the efficiency of the control software developed (MPC@CB) under Matlab. MPC@CB may be easily used for any other process and any constrained control problem.

1. Introduction

Freeze drying is a separation process in biotechnology, food and pharmaceutical industry, frequently used to stabilize and preserve the products. Compared with conventional drying techniques, freeze drying is generally considered to produce the highest quality dried products. The development of freeze-drying in industry today is limited by its actual cost and its use remains quite lower than the other techniques of drying. Indeed, the operating mode under vacuum and low

† Work partially supported by the AUF (Agence Universitaire Francophone).

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temperature involves important treatment times and thereafter a low productivity. Moreover, one very important parameter in the study of freeze-drying is the temperature of the product which must carefully be controlled during the primary drying stage: it cannot exceed the collapse limit of the cake structure or the melting temperature. The problem of optimal control of the primary and secondary drying stages of bulk solution freeze drying in trays to obtain a desired bound water content at a minimum time was formulated and solved by [1, 2]. The work described here is related to the model predictive control (MPC) [3] of the measured surface temperature evolution of the freeze dried product during the primary stage. A control software (MPC@CB) is used, allowing solving any other constrained optimal control problems for any processes. Temperature trajectory tracking results are presented here.

2. First Principle Model and Control Problem Formulation

In the controller, a dynamic behavior of the primary drying stage of the freeze drying process is needed: a multi-dimensional model based on fundamental mass and energy balance equations is used [1]. In this work, it is assumed [4]:

- One dimensional heat and mass transfer.
- The sublimation front is planar and parallel to the horizontal section of the vial.
- The gas phase inside the pores of the dry layer is composed only of pure water vapor.
- The value of the partial pressure of water vapor at the top of the dry layer is equal to the total pressure in the sublimation chamber.

The frozen region is considered to be homogeneous with uniform thermal conductivity, density and specific heat. During the primary drying, the vial contains two regions: a dry layer (index 1 in the model), in which the majority of water was sublimated and a frozen layer (index 2 in the model). These two areas are separated by a moving interface called the sublimation front described by *z=H(t)*. The mathematical model consists of the unsteady state energy balance in the dried and frozen regions:

$$\frac{\partial T_1}{\partial t} = \frac{k_{Ie}}{\rho_{Ie} c_{pI}} \frac{\partial^2 T_1}{\partial z^2} - \frac{c_{pg}}{\rho_{Ie} c_{pI}} \frac{\partial (N_t T_1)}{\partial z} \quad \text{for } t > 0, 0 < z < H(t) \qquad (1)$$

$$\frac{\partial}{\partial t}\left(\frac{p_w}{T_1}\right) = -\frac{R_{ig}}{\varepsilon M_w} \frac{\partial N_t}{\partial z} \quad \text{for } t > 0, 0 < z < H(t) \qquad (2)$$

$$\frac{dH}{dt} = \frac{-1}{\rho_2 - \rho_1} N_t \quad \text{for } t > 0, \mathrm{z} = H(t) \qquad (3)$$

$$\frac{\partial T_2}{\partial t} = \alpha_2 \frac{\partial^2 T_2}{\partial z^2} \qquad \text{for } t > 0, H(t) < z < L \tag{4}$$

where T_1 is the dried layer temperature, N_t is the total mass transfer flux, T_2 is the frozen layer temperature and p_w is the partial pressure of the water vapor. Based on the diffusion equations of Evans, the following simplified equation describes the dynamic of the mass transfer flux N_t:

$$N_t = N_w = -\frac{M_w k_1}{R_{ig} T_1 H}(p_{wH} - p_w^0) \text{ for } t > 0, 0 < z \leq H(t) \tag{5}$$

For equations (1-4), the initial conditions are $T_1(z,t) = T_2(z,t) = T^0$ for $t = 0, 0 \leq z \leq L$ and $p_w(z,t) = p_w^0$ for $t = 0, 0 \leq z \leq L$, and the boundary conditions:

$$-k_{Ie} \frac{\partial T_1}{\partial z} = \sigma F_{up}(T_{up}^4 - T_1^4) \text{ for } t > 0, z = 0 \tag{6}$$

$$k_{II} \frac{\partial T_2}{\partial z} - k_{Ie} \frac{\partial T_1}{\partial z} + (\rho_{II} c_{pII} T_2 - \rho_I c_{pI} T_1) \frac{dH}{dt} = -\Delta H_s N_t \text{ for } t > 0, z = H(t) \tag{7}$$

$$k_{II} \frac{\partial T_2}{\partial z} = h_v (T_{lp} - T_2) \text{ for } t > 0, z = L \tag{8}$$

where the process manipulated variables are the lower and upper heating plate temperatures $T_{lp}(t)$ and $T_{up}(t)$, which affect significantly the heat and mass transfer mechanisms of the freeze drying process in vials. The manipulated variable $T_{control}(t)=T_{lp}(t) = T_{up}(t)$ tuned online by the controller has to stay in the following set:

$$T_{\min} \leq T_{control}(t) \leq T_{\max} \tag{9}$$

3. Process Control Strategy

The control strategy used here is the model-based predictive control (MBPC) [3]. Since its first development at the early 70's, many MPC concepts have appeared and after the PID, MPC has become the second control paradigm in the history of control. Thousands of industrial applications of MPC exist today, for example in the chemical and petrochemical industries. MPC consists of solving an optimization problem formulated into the future. Constraints (such as manipulated variables physical limitations or operating procedures or safety reasons…) may be explicitly specified into this formulation. In this control structure, a model aims to predict the future behavior of the process and the best one is chosen by an optimal tuning of the manipulated variables. This procedure is repeated at each sampling time with the update of the process measurements.

In previous real applications [5], it has been shown how the current special partial differential equation (PDE) model MPC framework may be used for the control of such PDE systems, in spite of the relatively large size and non-linearity of the model state computed during the optimization, modelling errors and uncertainties. The control problem is a general optimization problem over a receding horizon N_p where the cost function J_{tot} to be minimized reflects any control problem J (trajectory tracking, processing time minimization, energy consumption minimization …) and where any constraints on measured or estimated output may be explicitly specified by J_{ext}. Since the problem is solved numerically, a mathematical discrete time formulation is given [5]:

$$\min_{p} \quad J_{tot}(p) = J(p) + J_{ext}(p) \tag{10}$$

where:

$$J_{tot}(p) = \sum_{j=k+1}^{j=k+Np} h(y_{ref}(j), y_p(k), y_m(j), u(p(j))) \tag{11}$$

where k (resp. j) is the actual (resp. future) discrete time index, y_{ref} describe the specified constrained behavior for the process measure y_p, y_m is the continuous model output in the future. The unconstrained optimization argument is p: it is obtained from a simple hyperbolic transformation of the magnitude and velocity constraints specified for the manipulated variable u [5]. The optimizer argument is now an unconstrained argument and any unconstrained optimization algorithm may be used to solve this on-line penalized optimization problem: widely known and used for its robustness and convergence properties, the Levenberg-Marquardt's algorithm is used.

4. Control Software: Main Features of MPC@CB

Based on the Levenberg-Marquardt's algorithm [5], the codes of the MPC@CB software[†] have been written with Matlab. It allows realizing the MPC under constraints of a continuous process. The originality of these codes is first the ease of their use for any continuous process, through the user files (where model equations have to be specified), synchronized by few main standards files (where the user has to make few (or no) changes). The model has to be given under the form:

$$\begin{cases} \dfrac{ds}{dt} = f(s,u) \\ y = g(s) \end{cases} \tag{12}$$

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i.e., there are any number of states variable *s* in this model, it may be linear or non linear, time variant or time invariant, based on ordinary differential equations and/or PDE.

Another original feature of the software is the straightforward resolution of various model based optimal control problems through few tuning parameters: trajectory tracking problem, operating time minimization problem, with or without the output constraint. The user may specify any other optimal problem.

The other originality is the method used to develop the codes: it is very easy to introduce new parts in the code, such as: user defined problem, handle SIMO, MISO or MIMO model (where: S means single, M means multiple, I means input and O means output), and introduce a software sensor (observer).

5. Simulation Results

The optimal control problems is the trajectory tracking of a given reference for the measured temperature $T_2(z=L,t)$. During the drying, the MPC@CB tunes automatically the temperature $T_{control}(t)=T_{up}(t)=T_{lp}(t)$ such that the measured temperature $T_2(z=L,t)$ tracks as best as possible the given temperature reference. Figure 1 shows that the measured temperature tracks very well its prescribed time trajectory, due to the online optimal tuning of the manipulated variable $T_{control}(t)$ (Figure 2) by MPC@CB, and under input constraints (9).

6. Conclusion

A model predictive control framework has been used in a general control software named MPC@CB. It has been shown how a specified reference trajectory of one of the drying characteristics may be tracked online during the primary drying, due to the optimal tuning of the manipulated variable by the control software. Current developments are concerned with the minimization of the primary drying time under constraints. Moreover, the MPC@CB software presented here may be easily used for any other process, for any constrained control problem.

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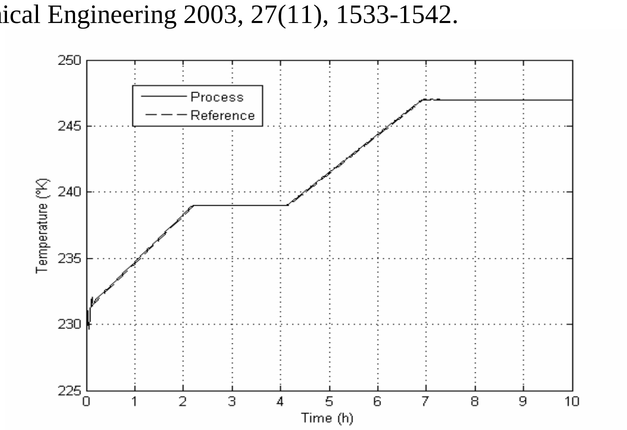

Figure 1. Temperature trajectory tracking results during the primary stage.

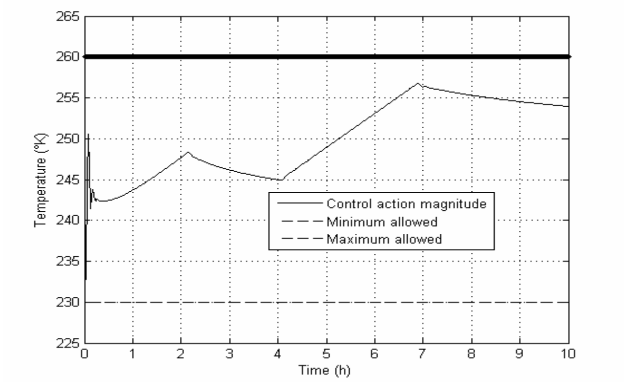

Figure 2. Constrained control temperature tuned by the MPC@CB software during the primary stage.