NONLINEAR MULTIPLE MODEL PREDICTIVE CONTROL IN A FED-BATCH REACTOR

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Abstract: In this work we study the use of nonlinear model predictive control for the control of fed-batch processes. The main idea is to use composite nonlinear models consisting of multiple linear models that are identified and interpolated. The approach is illustrated by a simulation study of a fed-batch process for the synthesis of hexyl monoester maleic acid.

Keywords: Batch control, Predictive control, Identification, Nonlinear systems, Optimization problems.

1. INTRODUCTION

In this work we study the use of nonlinear model predictive control (**NMPC**) for the control of batch and fed-batch processes. Such processes are common in industries where the linear model predictive control (**LMPC**) strategy is well accepted. However, the highly nonlinear nature of most batch and fed-batch processes suggest that performance will be lost when using **LMPC** rather than **NMPC**.

Industrial implementations of **LMPC** rely on most cases on experimental models that are derived using designed experiments and systems identification. For the application of **NMPC**, the development of a nonlinear prediction model is a major bottleneck, in addition to the design of nonlinear state estimators and implementation of reliable nonlinear programming algorithms for the real-time optimization. Any practical **NMPC** implementation must resolve the above mentioned problems. In this work we focus our attention to **NMPC** of batch processes, and like (Foss *et al.* 1995), (Townsend *et al.* 1998), (Trierwiler and Secchi 1998), (González Santos *et al.* 1999), (Mollov *et al.* 1998), (Roubos *et al.* 1998) we investigate the use of a composite global model based on multiple local models as an underlying model representation in cases when a global nonlinear model is not readily available. Such models offer the advantage that they are still transparent in the sense that their structure posses a useful interpretation for both model development and validation.

2. NONLINEAR MPC OF BATCH PROCESSES

Optimization problems in batch or fed batch processes are dynamic problems involving highly nonlinear process models. This problem can be formulated, in general form, as:

$$min_{u,t_f} J(x(t_f), u, t_f) \qquad (1)$$

subject to

$$\dot{x} = f(x, u, t), x(t_o) = x_o \tag{2}$$

$$h(x, u, t) \leq 0 \tag{3}$$

where x are states variables, u are control inputs defined on the time interval t_o to t_f, and h represents state and input constraints.

The objective is operate the process maximising an economic objective function J. J is a function of the states at the final time t_f and the final time itself. The resulting problem is a non-linear dynamic optimization problem, and (Rupppen *et al.* 1995), (Luus and Okongwu 1999), (Loeblin *et al.* 1999) and (Fournier *et al.* 1999) describe similar formulations. The optimization problem is defined on a batch time where t_f defines the end of the batch, and this variable could be optimised too. At each sampling time, the optimizer finds a future control input trajectory by optimizing over a prediction horizon that is an interval between actual time t, and the final batch time t_f.

The first sample of this input trajectory is applied to the plant, and the optimization is repeated at the next sample using the new states of the plant. Often, some states can not be measured and in this case it is necessary to introduce state estimators in this formulation, e.g. (Laksmanan and Arkun 1999).

3. MULTIPLE LOCAL MODELS

This section reviews a technique for developing composite non-linear models based on multiple local models, (Murray-Smith and Johansen 1997). Consider the problem of developing a state-space model of the form:

$$\dot{x} = f(x, u, t) \tag{4}$$

$$y = g(x, t) \tag{5}$$

where x is the state vector, u is the control input vector, and y is the measurement vector. When the system operates within a small operating regime, a simple (possibly linear) *local model* structure:

$$\dot{x} = f_i(x, u, p_i, t) \tag{6}$$

$$y = g(x, p_i, t) \tag{7}$$

parameterized with the vector p_i will describe the system dynamics, provided the nonlinearities are smooth. The local model structure will be valid within this particular operating regime, and more or less invalid outside this regime. The choice of which variables, z, to use to characterize the operating regimes will be highly problem dependent. Typically, z will contain elements of the state and input vectors, i.e. given by a function $z = H(x, u)$, but can also contain other model variables. The full range of operation is the set of operating points Z. An operating regime is defined as a subset Z_i where the local model structure above is an adequate description of the system.

Next, assume that for the local model structure above there exists a local model validity function $\rho_i(z) \geq 0$ that is designed such that its value is close to one for operating points z where the local model structure above is a good description of the system, and close to zero otherwise. If the system's operating range Z is decomposed into N operating regimes, $Z_1, \ldots, Z_N$, and local model structures and local model validity functions for each operating regime are developed, then the following interpolation gives a global model structure:

$$\dot{x} = \sum_{i=1}^{N} f_i(x, u, p_i, t) w_i(z) \tag{8}$$

$$y = \sum_{i=1}^{N} g(x, p_i, t) w_i(z) \tag{9}$$

$$w_i(z) = \frac{\rho_i(z)}{\sum_{j=1}^{N} \rho_j(z)} \tag{10}$$

The interpolation function w_i is a normalization of the model validity function, and has the property:

$$\sum_{i=1}^{N} w_i(z) = 1 \tag{11}$$

for all z. To guarantee a complete global model, it must be assumed that at any operating point z, at least one local model validity function is non-zero. With this framework, the modeling problem consists of the following major tasks:

(1) First, decompose the system's operating range into a number of operating regimes that completely cover the interesting range of operation. Such a decomposition can often be found by using an elementary understanding of the mechanisms in the system.
(2) Second, for each operating regime, a local model structure must be developed. In addition, local model validity functions must be designed. However, this is usually a quite straightforward task when the decomposition into regimes has been accomplished.
(3) Third, the unknown parameters $p_1, \ldots, p_N$ must be identified. If the local model structures are linearly parameterized, the local model validity function do not contain unknown parameters. Standard system identification tools can be applied. Since the model is nonlinear it is particularly important with

informative data that covers all operating regimes with local models that contain unknown parameters.

4. SIMULATION EXAMPLE

Multiple local models that describe the non-linear dynamics are obtained and validated with ORBIT, a MATLAB based tool for operating regime based modelling and identification, (Johansen and Foss 1998), in a realistic simulation study.

4.1 *System description*

The simulated true system model describe a synthesis of hexyl monoester maleic acid according to maleic anhydride and hexanol reaction. In fed-batch operation, reactant A (maleic anhydride) is first melted; then reactant B (hexanol) is added at a regulated rate so that the heat generated is matched by the cooling capacity. The following state-space model is used to simulate the true system (Chang and Hseih 1995):

$$\dot{C}_a = -\frac{C_a U_1}{V_r} - kC_aC_b \tag{12}$$

$$\dot{C}_b = \frac{(C_{bl} - C_b)U_1}{V_r} - kC_aC_b \tag{13}$$

$$\dot{T} = -\frac{\Delta H}{\rho C_p}kC_aC_b - (T - 327)\frac{U_1}{V_r} - U_2(T - 327) \tag{14}$$

$$\dot{V}_r = U_1 \tag{15}$$

$$k = k_o \exp(-12628/T) \tag{16}$$

Input variables are reactive flow rate U_1 and cooling fluid flow rate U_2. State variables are reagent A (maleic anhydride) and reagent B (hexanol) concentrations C_a, C_b, reactor temperature T_r and reactor volume V_r. Feed flow of reagent B has concentration C_{bl}. Figure 1 shows three system trajectories corresponding to different constant inputs, when the batch time is equal to $t_f = 6700$ s. In the upper plot, $U_1 = 1.0 \cdot 10^{-5}$ and $U_2 = 1.0 \cdot 10^{-5}$, while in the middle plot, $U_1 = 0.355 \cdot 10^{-3}$ and $U_2 = 2.0 \cdot 10^{-5}$, and in the lower plot $U_1 = 1.0 \cdot 10^{-2}$ and $U_2 = 253 \cdot 10^{-6}$. At higher feed rates, greater than $U_1 = 0.355 \cdot 10^{-3} m^3/s$, the maximum allowable temperature ($373K$) is exceeded. Model parameters and nominal initial state of fed-batch reactor appear in Table 1.

Table 1. Model parameters

Parameter	Value	Units
C_{bl}	9.7	$kmol/m^3$
k_o	$1.37 * 10^{12}$	$m^3/kmols$
$\frac{\Delta H}{\rho C_p}$	16.92	$m^3 K/kmol$
C_{ao}	10.1	$kmol/m^3$
C_{bo}	0.0	$kmol/m^3$
T_o	328	K
V_{ro}	2.2	m^3
$U_{1,min}$	0	m^3/s
$U_{1,max}$	0.01	m^3/s
$U_{2,min}$	0	s^{-1}
$U_{2,max}$	0.000253	s^{-1}

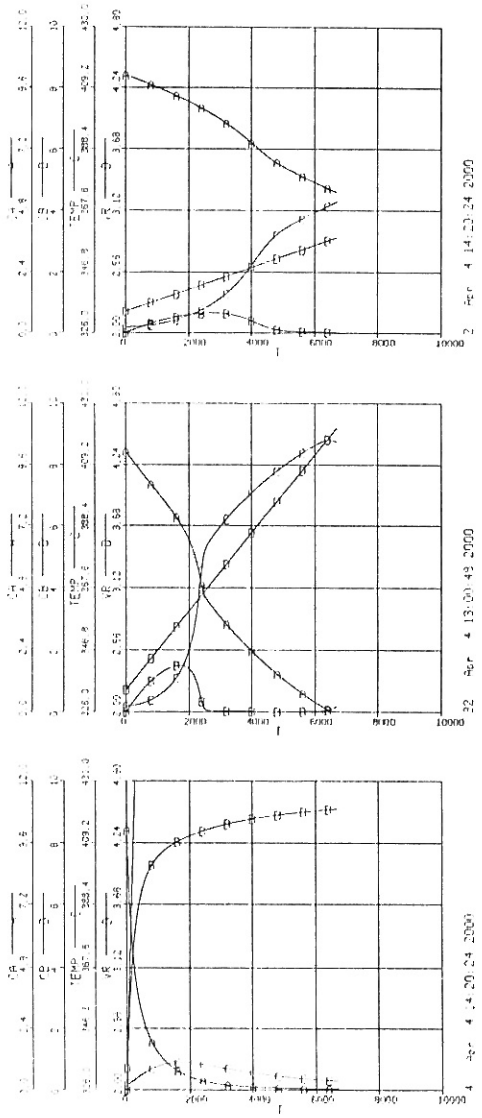

Fig. 1. Typical state trajectories.

4.2 *Modeling and Identification*

All the local models are chosen to have the same linear structure:

$$x(t+1) = a_i + A_i x(t) + B_i u(t) \tag{17}$$

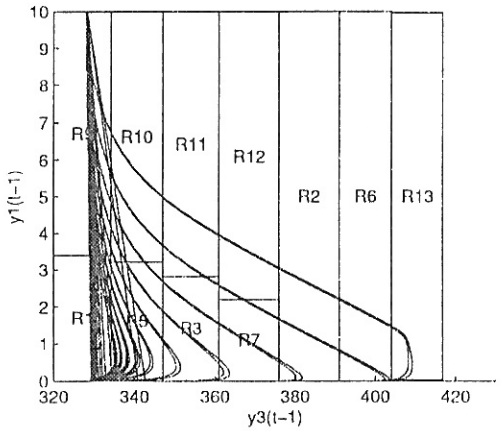

Fig. 2. Operating regimes.

where $x = (C_a, C_b, T_r, V_r)$, $u = (U_1, U_2)$, a_i is a vector of unknown parameters and A_i and B_i are system matrices of unknown parameters. For different initial conditions and input trajectories a number of representative batch simulations realized and identification data were generated.

Using ORBIT (Johansen and Foss 1998) we identified and validated a composite model consisting of 11 operating regimes with local linear models within each regime. The operating regimes are characterized using the variables T_r and C_a as shown in Figure 2.

Notice that the equation for the volume (15) was not identified since it was known a priori.

4.3 *Model Predictive Control*

The objective is to obtain a final conversion of product B concentration to product A concentration in 99 %. The optimization problem is formulated as:

$$min_{U_1(t),U_2(t)} J = (conv(t_f) - 99\%)^2 \qquad (18)$$

subject to the model equations (12),(13),(14),(15) and (16) and the additional constraints:

$$U_1(t) \in [0.0, 0.01] \qquad (19)$$

$$U_2(t) \in [0.0, 0.000253] \qquad (20)$$

$$T \leq 373K \qquad (21)$$

$$V_r \leq 4.7\ m^3 \qquad (22)$$

Conversion is calculated as

$$conv(t_f) = 1 - \frac{V_r(t_f)C_a(t_f)}{V_r(t_o)C_a(t_o)} \qquad (23)$$

where t_o is the start time of the batch.

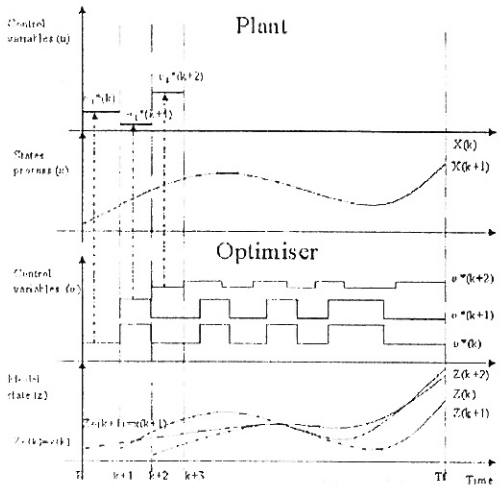

Fig. 3. Nonlinear optimization problem strategies.

The input constraints (19), (20) and the volume constraint (22) represents physical limitations, while (21) is an upper bound on the allowed temperature.

The trajectories are optimized from time t to the batch end time t_f, which nominally equals 6700 seconds. The sampling interval of the controller is $\Delta T = 100$ seconds.

At each sampling time, states are measured and above optimization problem was resolved in order to determine the optimum inputs to reach the objective. Figure 3 illustrates this procedure. The first value of the input trajectories were applied to the plant and the procedure is repeated at the next sample.

We consider two cases:

- NMPC using the perfect model in the optimization for prediction.
- MMPC (multi-model predictive control) where the identified composite model is used for prediction in the optimization.

In both cases, the criterion (18) is minimized using **e04jbc** NAG quasi-Newton algorithm, (NAG.Ltd 1996).

4.4 *Results and discussion*

The achieved cost (18) are summarized in Table 2 for three different initial conditions. Figures 4, 6, 8 and 10 show simulation results with NMPC. Figures 5, 7, 9 and 11 show simulations results with MMPC. These figures correspond to first simulation.

Table 2 also shows the final batch time. Results with MMPC show good results. The stop condition is when the volume V_r reaches the maximum capacity of reactor, due to, final time is different for every simulation. Constraint (21) was realized

Table 2. Achieved cost

Exp	NMPC	t_f	MMPC	t_f
1	0.9998	6087.5	0.9915	2120
2	0.9909	4621.1	0.9828	2910
3	0.9853	3730.1	0.9710	4210

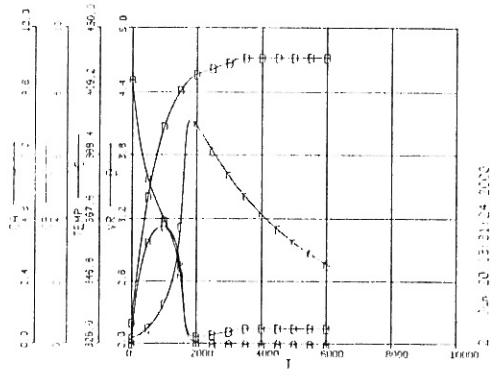

Fig. 4. Concentration A and B products, temperature and volumen with NMPC Results

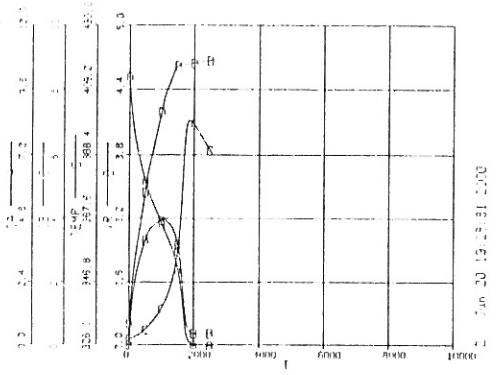

Fig. 5. Concentration A and B products, temperature and volumen with MMPC Results

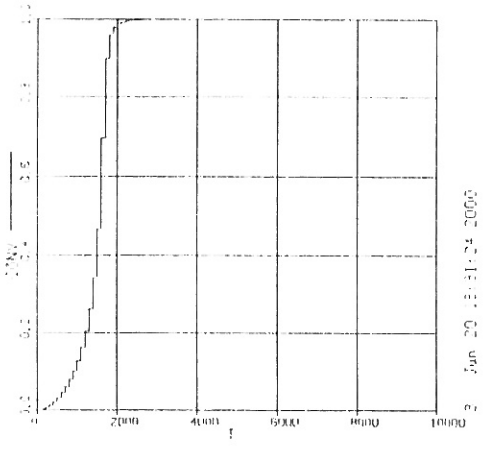

Fig. 6. Conversion achieved with NMPC Results

as a *soft* penalty function. The upper temperature of this reaction is less critical than for other reactions. This reason explains why violation in upper limit was permitted as show figures 4 and 5. Initial conditions are the same, U_1 is $0.008m^3/s$ and

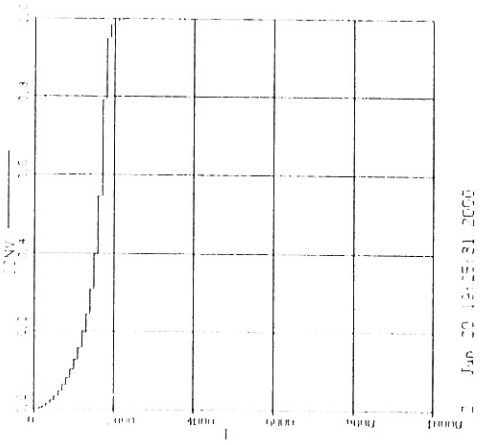

Fig. 7. Conversion achieved with MMPC Results

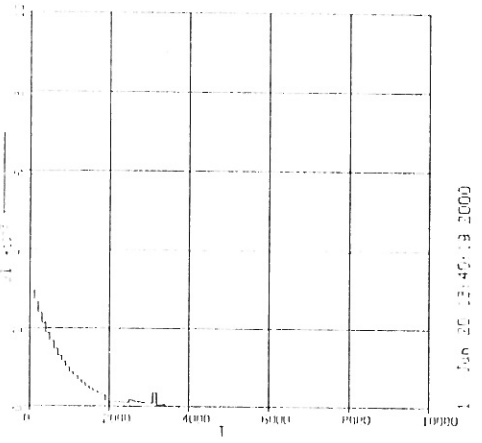

Fig. 8. Reactive flow input with NMPC Results

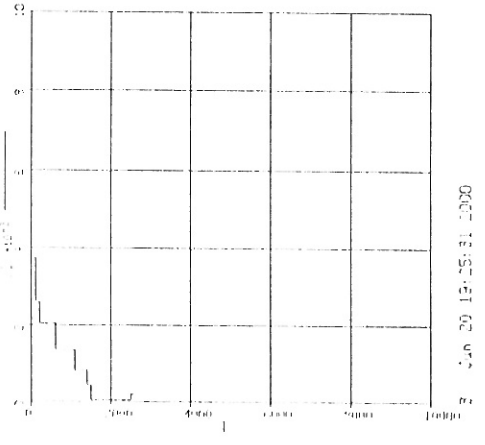

Fig. 9. Reactive flow input with MMPC Results

U_2 is $0.000253s^{-1}$ although variables are changed for the controller in first sampling time as show figures 8, 9, 10 and 11.

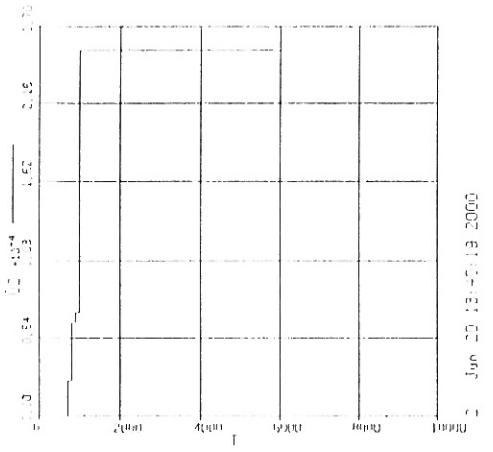

Fig. 10. Cold flow input with NMPC Results

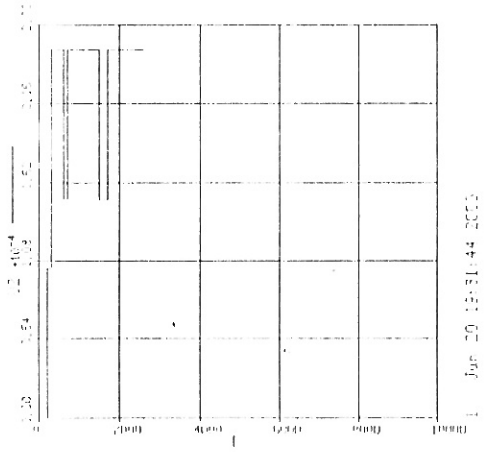

Fig. 11. Cold flow input with MMPC Results

5. CONCLUSIONS

This investigation showed that the operating regime based modeling framework can be used as a means for modelling batch and fed-batch processes from experimental data. Simulation experiments show that multiple model predictive control might be a useful alternative in these processes.

Modeling and identification procedure suggest that critical part is characteristic variable selection and regimes splitting. Estimation aspect is obviously important from a practical point view, it has not been considered here because we supposed all states measured.

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