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# Advanced process control of pantolactone synthesis using nonlinear model predictive control (NMPC)

Calin Cormos *, Serban Agachi

"Babes – Bolyai" University, Faculty of Chemistry and Chemical Engineering, 11 Arany Janos Street, RO-400028, Cluj – Napoca, Romania, Tel: +40264593833, Fax: +40264590818, E-mail: cormos@chem.ubbcluj.ro, sagachi@chem.ubbcluj.ro

## Abstract

In this paper, the discontinuous synthesis of racemic pantolactone has been described. The chemical steps of the synthesis take place in two stirred tank reactors, operated batchwise. The chemical reactions are highly exothermic. For a good quality of the product, the reactor temperature must be maintained between 12 – 14°C.

The control of the reactor temperature was studied in two different situations, first using Proportional – Integral – Derivative (PID) controllers and second using a Nonlinear Model Predictive Control (NMPC). The aim of this process control study was to reduce the cooling agent consumption and to improve the quality of the product by better reactor temperature control. The pantolactone synthesis process was modeled and simulated using MATLAB / SIMULINK software package.

It was demonstrated that using PID controllers the cooling agent consumption can be reduced with 10 % (comparing to real plant operation), but the reactor temperature control could be improved. In case of using an advanced reactor temperature control (model predictive control), the cooling agent consumption can be further reduced with 8 % and the temperature of the reactor is very well controlled.

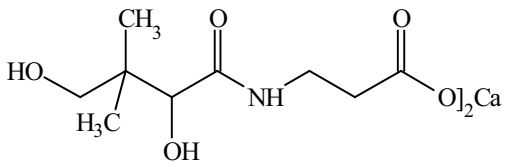
The applications developed for racemic pantolactone synthesis were validated by comparison with data collected from real plant operation and can be used to improve real plant operation.

**Keywords:** Modeling, simulation, model predictive control, batch processes

## 1. Introduction

Calcium pantothenate is one of the most used pro-vitamins in the therapy for the human beings and for the veterinary use. Pantothenic acid is a vitamin from the complex of vitamins B; it plays an important role in the metabolism, its biological active form is Coenzyme A (Neamtu, 1996).

The chemical formula of calcium pantothenate is presented below:



In the synthesis of calcium panthotenate, pantolactone (α-hydroxy-β,β-dimethyl-γ-butyrolactone) and beta-alanine are used as starting materials.

In this paper the synthesis of racemic pantolactone has been described. The chemical steps of the synthesis take place in two stirred tank reactors operated batchwise (Distiler and Goetze, 1980).

The first step of the synthesis consists in the reaction between formaldehyde and isobutyraldehyde, the reaction is catalyzed by sodium hydroxide. The reaction is highly exothermic ($\Delta H_1$ = -36.45 kJ/mole). For a good control of the temperature, the reactor is equipped with an external jacket and two internal coils. As cooling agent, a mixture of methanol and ethylene glycol, with a low temperature (-12°C), is used. The reactor temperature must be maintained under 14°C. The control of the reactor temperature is achieved both using the sodium hydroxide flow added into the reactor and the cooling agent flows (from the jacket and the coil of the reactor). The first reaction product is α,α-dimethyl-β-hydroxy-propionic aldehyde (oxymethyle).

The second step of the synthesis consists in the reaction between α,α-dimethyl-β-hydroxy-propionic aldehyde and a sodium cyanide solution. The reaction is highly exothermic ($\Delta H_2$ = -84.4 kJ/mole). The control of the reactor solution temperature (12 – 14°C) is achieved controlling sodium cyanide solution flow and cooling agent flows (from the jacket and the coil) as manipulated variables. The second reaction product is α,γ-dihydroxy-β,β-dimethyl-butyronitrile (nitrile).

The α,γ-dihydroxy-β,β-dimethyl-butyronitrile solution is then transferred in a different stirred tank reactor (operated batchwise) and hydrolyzed in acidic condition in order to obtain an aqueous racemic pantolactone solution.

## 2. Modeling and simulation of the synthesis process

The mathematical model of α,γ-dihydroxy-β,β-dimethyl-butyronitrile synthesis uses mass and energy balances for the reactor. During the synthesis, the parameters analyzed are: reactor mass (M), reactor volume (V), temperatures for reaction mass (T), jacket-cooling agent ($T_{ag}$) and coils-cooling agent ($T_{ags}$) and molar concentrations of the different chemical species ($C_i$). The model of the pantolactone synthesis is nonlinear.

Because the mathematical equations for the each step are similar, below are presented only the equations for the second reaction, between sodium cyanide solution and α,α-dimethyl-β-hydroxy-propionaldehyde (Cormos and Agachi, 2000).

$$\frac{dM}{dt} = F_{NaCN}\rho_{NaCN} \tag{1}$$

$$\frac{dV}{dt} = F_{NaCN} \tag{2}$$

$$\begin{aligned}\frac{dT}{dt} = \frac{1}{(MCp)}(&F_{NaCN}\rho_{NaCN}Cp_{NaCN}T^0 - F_{NaCN}\rho_{NaCN}Cp\,T - \\ &- K_t A_t (T - T_{ag}) - 2K_{ts}A_{ts}(T - T_{ags}) - \\ &- \Delta H_2\, k_2\, C_{NaCN}\, C_{oxymethyle}\, V - \Delta H_1\, k_1\, C_{NaOH}\, C_{IBA}\, V)\end{aligned} \tag{3}$$

$$\frac{dT_{ag}}{dt} = \frac{F_{ag}}{V_m}(T^0{}_{ag} - T_{ag}) + \frac{K_t A_t}{V_m \rho_{ag} Cp_{ag}}(T - T_{ag}) \quad (4)$$

$$\frac{dT_{ags}}{dt} = \frac{F_{ags}}{V_{ms}}(T^0{}_{ags} - T_{ags}) + \frac{K_{ts} A_{ts}}{V_{ms} \rho_{ag} Cp_{ag}}(T - T_{ags}) \quad (5)$$

$$\frac{dC_{IBA}}{dt} = -\frac{F_{NaCN} C_{IBA}}{V} - k_1 C_{NaOH} C_{IBA} \quad (6)$$

$$\frac{dC_{NaOH}}{dt} = -\frac{F_{NaCN} C_{NaOH}}{V} + k_2 C_{NaCN} C_{oxymethyle} \quad (7)$$

$$\frac{dC_{NaCN}}{dt} = \frac{F_{NaCN}(C^0{}_{NaCN} - C_{NaCN})}{V} - k_2 C_{NaCN} C_{oxymethyle} \quad (8)$$

$$\frac{dC_{oxymethyle}}{dt} = -\frac{F_{NaCN} C_{oxymethyle}}{V} - k_2 C_{NaCN} C_{oxymethyle} + k_1 C_{NaOH} C_{IBA} \quad (9)$$

$$\frac{dC_{nitrile}}{dt} = -\frac{F_{NaCN} C_{nitrile}}{V} + k_2 C_{NaCN} C_{oxymethyle} \quad (10)$$

*Table 1. Parameters of pantolactone synthesis model (Cormos, 2004 and Frost, 1961)*

| | | |
|---|---|---|
| $T^o = 288$ K | $A_{ts} = 1.5$ m$^2$ | $\Delta H_1 = -36450000$ J/kmole |
| $T^o_{ag} = 260$ K | $\rho_{NaCN} = 1150$ kg/m$^3$ | $\Delta H_2 = -84400000$ J/kmole |
| $T^o_{ags} = 260$ K | $\rho_{ag} = 965.64$ kg/m$^3$ | $C^0_{NaCN} = 6.122$ kmole/m$^3$ |
| $K_t = 443$ W/m$^2$ K | $Cp = 2900$ J/kg K | $C^0_{NaOH} = 7.5$ kmole/m$^3$ |
| $K_{ts} = 817$ W/m$^2$ K | $Cp_{NaCN} = 3414.01$ J/kg K | $V_{ms} = 0.1$ m$^3$ |
| $A_t = 10$ m$^2$ | $Cp_{ag} = 2231.13$ J/kg K | $V_m = 0.5$ m$^3$ |
| $k_1 = A_1 \exp(-E_{a1}/RT)$ | $A_1 = 10^{11}$ m$^3$/kmole s | $E_{a1} = 73.24$ kJ/mole |
| $k_2 = A_2 \exp(-E_{a2}/RT)$ | $A_2 = 2*10^{11}$ m$^3$/kmole s | $E_{a2} = 75$ kJ/mole |

The nonlinear model described above was simulated using MATLAB-SIMULINK software package (the model was implemented as an S-function).

The control of the reactor temperature was studied in two different situations. The first study was made using Proportional – Integral – Derivative (PID) controllers to control the reactor temperature. For this purpose, three PID controllers were used (for sodium hydroxide solution flow, sodium cyanide solution flow and cooling agent flow).

The second study was made using a MPC controller. The MPC controller was implemented from SIMULINK library (MPC Toolbox). In case of reactor temperature control using model predictive control, two disturbances of the process (one measured and one unmeasured) were simulated. The measured disturbances were variations, in ramp and sinusoidal modes, of sodium hydroxide and sodium cyanide inlet concentrations (feedforward compensation). The unmeasured disturbance was variation, in a ramp mode, of the cooling agent inlet temperature (feedback compensation).

## 3. Results and discussions

In the figure 1 is presented the application for simulation of pantolactone synthesis using three PID controllers (Cormos, 2004).

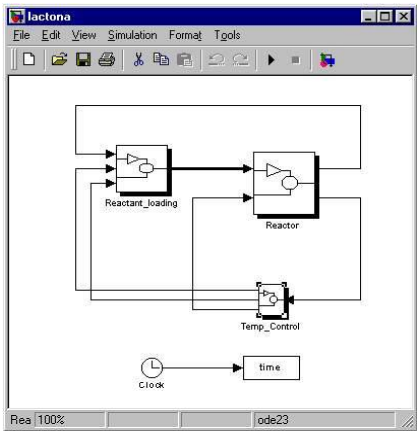



*Figure 1. Simulation of pantolactone synthesis using PID controllers*

In the figures 2 and 3 are presented the variations of chemical species concentrations and temperatures (reaction mass and cooling agent) during the synthesis.

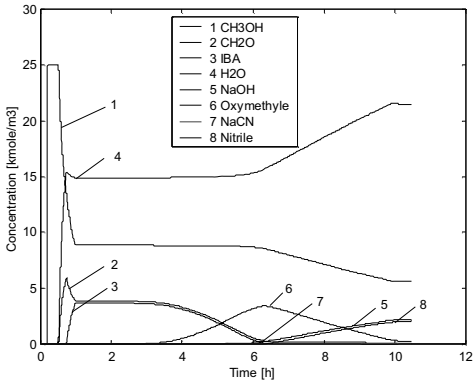



*Figure 2. Concentrations variation*

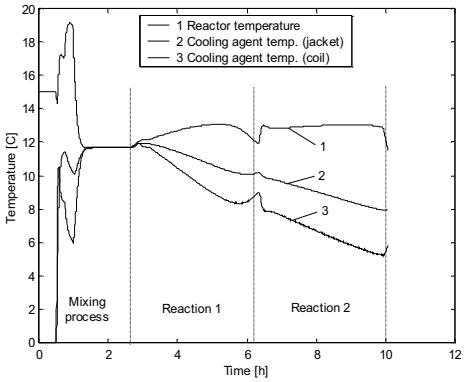



*Figure 3. Temperatures variation*

The real plant has only two PID control systems for the reactor temperature using sodium hydroxide and sodium cyanide flows as manipulated variables.

From the comparison of the simulation results (3 PID controllers) with real plant operation data, a close similarity can be observed. This fact validates the application developed for simulation of pantolactone synthesis (Cormos, 2004).

Also, it was calculated that the introduction of one supplementary temperature control systems leads to a cooling agent economy with 10 %. The annual cooling agent economy, obtained by introduction of third PID, is $2,500 (Cormos and Agachi, 2003).

In addition, the introduction of supplementary temperature control systems leads to a better reactor temperature control in comparison with the present situation used in practice, with benefic consequences on the quality of the product.

In the figures 4 and 5 are presented the applications for simulation of pantolactone synthesis using a MPC controller. In these applications two disturbances of the process were implemented, one measured (sodium hydroxide and sodium cyanide inlet concentrations) and one unmeasured (cooling agent inlet temperature).

The MPC applications use, for prediction of the system behaviour, a linearized model of the synthesis reactor. The sampling time was set to 1 min., control horizon to 1 and prediction horizon to 10. The weights on manipulated variables rates were set to 0.2, weight on controlled output variable (reactor temperature) was set to 2 and the rest of output variables weights were set to 0 (no control). The reference temperature of the reaction mass was set to 13°C for the first reaction and to 12°C for the second reaction.

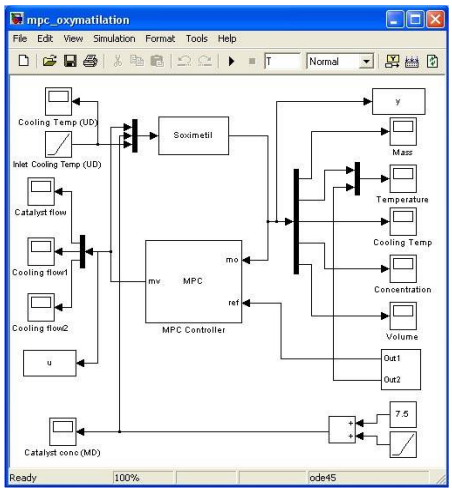



*Figure 4. MPC for oxymethylation process*

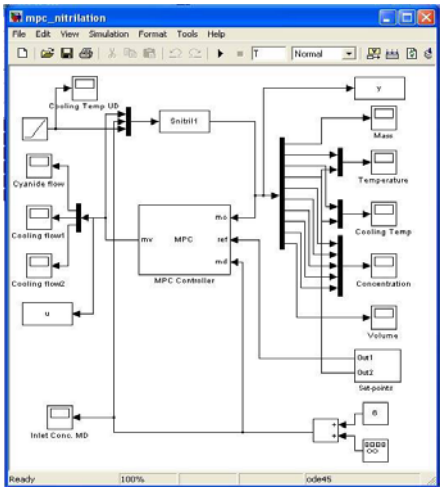



*Figure 5. MPC for nitrilation process*

The variations of chemical species concentrations, reaction mass and reaction volume in case of using a MPC controller are similar with the variations of these parameters in case of using PID controllers. In the figures 6 and 7 are presented the variations of temperatures (for reaction mass and cooling agent from jacket and coils) during the oxymethylation (figure 6) and nitrilation (figure 7) processes.

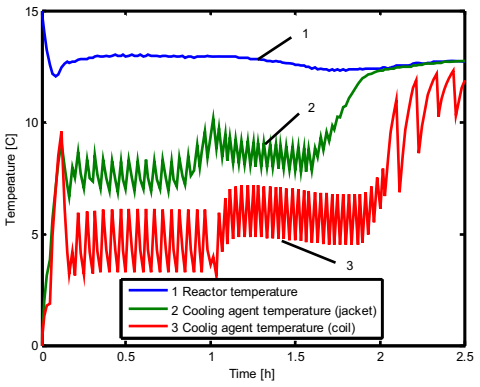



*Figure 6. Temp. variation during oxymethylation*

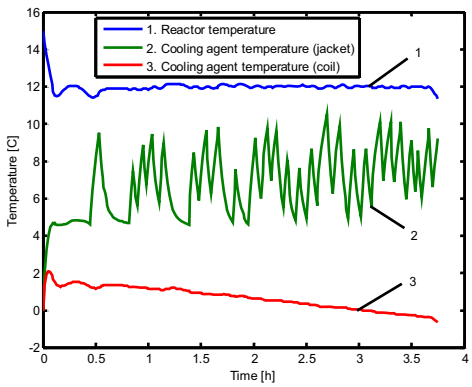



*Figure 7. Temp. variation during nitrilation*

Comparing the simulation results in case of using 3 PID controllers with simulation results in case of using a MPC controller it was calculated that the in the second case the cooling agent consumption is lower with 8 % comparing with the first case. The value of additional annual cooling agent economy is $2,000.

Also, the reactor temperature is better controlled in case of a MPC controller even if the process disturbances are present. This fact has benefic consequences on the quality of the pantolactone and in the end on the quality of calcium pantothenate.

## 4. Conclusions

In this paper the discontinuous synthesis of racemic pantolactone was presented. The mathematical model of the synthesis process was modeled and simulated using MATLAB / SIMULINK software package.

The control of the reactor temperature was studied in two different situations. In the first case Proportional – Integral – Derivative (PID) controllers were used. The second case uses MPC controller implemented as a SIMULINK block (MPC Toolbox, version 2). The aim of this process control study was to reduce the cooling agent consumption, to study the disturbance rejection and to improve the quality of the product by better reactor temperature control.

It was demonstrate that using PID controllers the cooling agent consumption can be reduced with 10 % comparing to the real plant operation, but the reactor temperature control stands for further improvement. In case of using an advanced temperature control (model predictive control), the cooling agent consumption can be further reduced with 8 % and the temperature of the reactor is very well controlled.

The model proved to be a reliable tool for analyzing pantolactone synthesis process. Using the model of the synthesis process and the simulation results (for different operational conditions) very valuable information can be obtained for the real plant operation (temperature control improvement, reduction of cooling agent consumption, disturbance rejection, investigation of different control strategies etc.).

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### 6. Acknowledgements


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