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MODELING AND SIMULATION OF SODIUM PANTOTHENATE SYNTHESIS USING CHEMCAD

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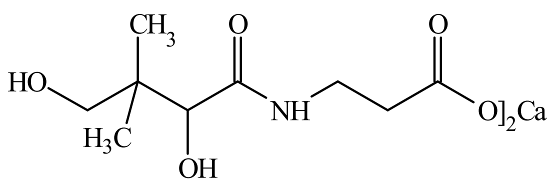
ABSTRACT

In this paper the mathematical model and the simulation for the discontinuous synthesis of racemic sodium pantothenate (an intermediary product in the synthesis of racemic calcium pantothenate) have been described. The chemical step of the synthesis takes place in a continuous stirred tank reactor (CSTR), operated batchwise. The synthesis reaction is reversible and highly exothermic. For a good quality of the product, the temperature of the solution from the reactor must be maintained between 13 – 15 °C. A control of reactor solution temperature was studied using a PID controller. The mathematical model of the process was simulated using ChemCAD 5.0 software package. From the simulation results very valuable information can be obtained regarding real plant operation.

KEY WORDS: Modeling, simulation, control, sodium pantothenate

1. INTRODUCTION

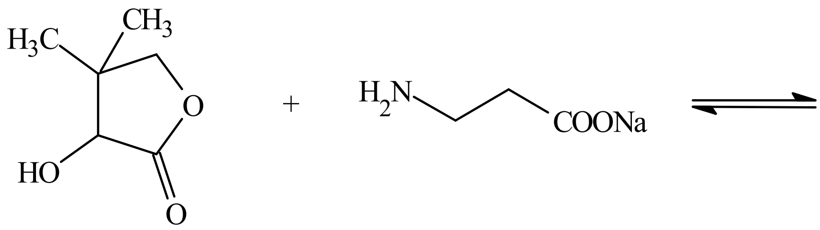
Calcium pantothenate is one of the most used pro-vitamins in the therapy for the human beings and for the veterinary use. Pantothenic acid is a vitamin from the complex of vitamins B; it plays an important role in the metabolism [1] (its biological active form is Coenzyme A). The chemical formula of calcium pantothenate is presented below:



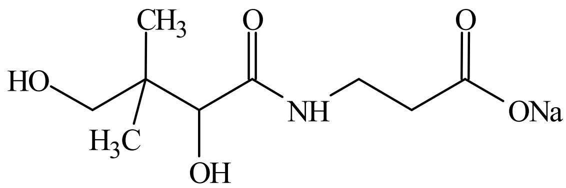
The synthesis of racemic calcium pantothenate is a complex process. The synthesis involves three major steps, the first step is the manufacture of pantolactone (α-hydroxy-β,β-dimethyl-γ-butyrolactone), the second step consists of the manufacture of sodium β-alaninate and in the final step of the synthesis these intermediaries are coupled resulting the final product [2].

Because the technology is very complex including a large category of operations, the mathematical models have been developed for the different steps of the synthesis. These mathematical models have been used to simulate the process, in which purpose ChemCAD software package has been employed. The goals of modeling and simulation of the processes were to find the best operating points, to try different control algorithms, to improve the energy consumption of the plant [3, 4, 5, 6].

In this paper, the mathematical model for the discontinuous synthesis of sodium pantothenate has been described. The chemical reaction is presented below:



Racemic pantolactone   Sodium β-alaninate



Sodium pantothenate

Sodium pantothenate synthesis from pantolactone and sodium β-alaninate is a reversible process. The synthesis takes place in a batch reactor. First step of the synthesis consists in the loading of sodium β-alaninate solution into the reactor. The sodium β-alaninate solution has a slightly sodium hydroxide excess (1 – 3%). After that, the reactor cooling is started and water is added in the reactor. The dilution process is exothermic. For a good control of the temperature the reactor is equipped with an external jacket. As cooling agent, a mixture of water and ethylene glycol, with a low temperature (-15^{o}C) is used. After the reactor mass temperature decreases below 12^{o}C, a pantolactone solution is added in the reactor. Pantolactone, added in the reactor, reacts with sodium β-alaninate and gives sodium pantothenate. The chemical reaction is highly exothermic (ΔH_r = -302.83 kJ/mole). In practice, the reactor temperature must be maintained under 15^{o}C (above this temperature secondary products could result). For the reactor temperature control, a Proportional – Integral – Derivative (PID) controller is used. The control of reactor temperature is achieved using the pantolactone flow added into the reactor or the cooling agent flow (as manipulated variables). The reaction product is sodium pantothenate, which then is used to obtain calcium pantothenate.

2. MODELING AND SIMULATION OF THE SYNTHESIS

The discontinuous synthesis of sodium pantothenate was modeled and simulated using ChemCAD 5.0 software package.

The parameters of the mathematical model for sodium pantothenate synthesis are presented in tables 1, 2 and 3 [2, 4, 7].

Table 1. Synthesis reactor parameters

Reactor volume	15 m^3
Jacket volume	0.8 m^3
Heat transfer area	30 m^2
Reactor diameter	2.6 m
Impeller diameter	1.8 m
Impeller speed	180 rpm
Motor power	10 kW

Table 2. Kinetic and thermodynamic parameters [4, 7]

Parameters	Direct reaction	Indirect reaction
Heat of reaction	-302,83 kJ/mole	302,83 kJ/mole
Kinetic data	$k_1 C_{Sodium\ \beta\text{-}alaninate} C_{Pantolactone}$	$k_{-1} C_{Sodium\ pantothenate}$
Frequency factor	2×10^{11} m^3/kmole · s	4×10^{10} s^{-1}
Activation energy	71,1 kJ/mole	75 kJ/mole

Table 3. Control system parameters [4, 7]

Parameters	Proportional band	Integral time	Derivative time
PID controller	150	5 min.	10 min.

The sodium pantothenate synthesis process was modeled and simulated in two different situations. The first situation considers a control of the reactor temperature using a PID controller and in the second situation no temperature control system is used.

The main window of the application for simulation of sodium pantothenate synthesis (with one PID controller for reactor temperature using pantolactone solution flow added into the reactor) is presented in the figure 1.

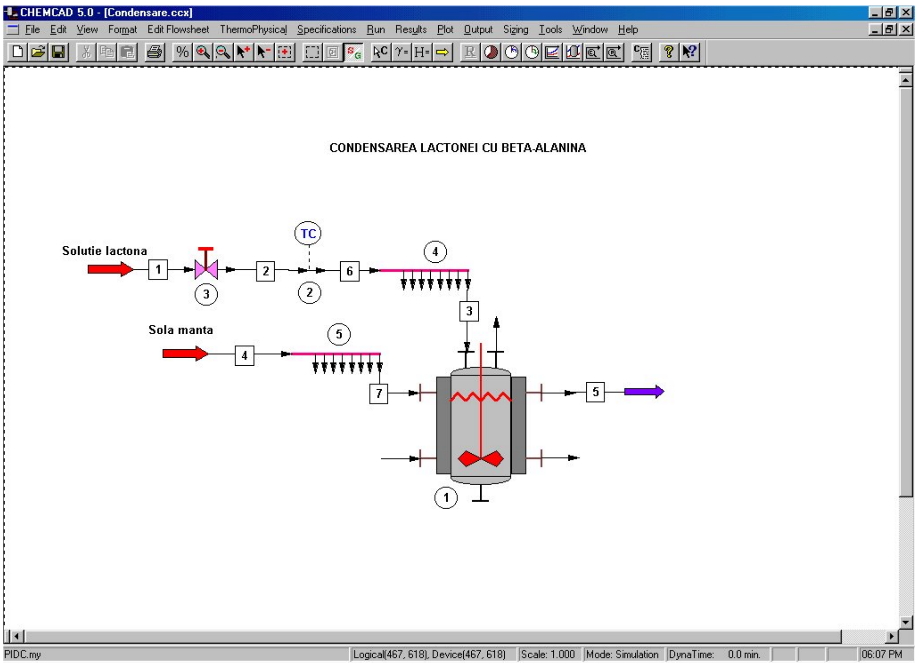


Figure 1. Simulation of sodium pantothenate synthesis using ChemCAD
1 – Synthesis reactor, 2 – PID controller, 3 – Control valve, 4,5 – Time switch

3. RESULTS AND DISCUSSIONS

The mathematical model of the sodium pantothenate synthesis process was simulated using ChemCAD 5.0 software package.

The variation of the chemical species concentrations from the reactor solution during the sodium pantothenate synthesis are presented in figure 2.

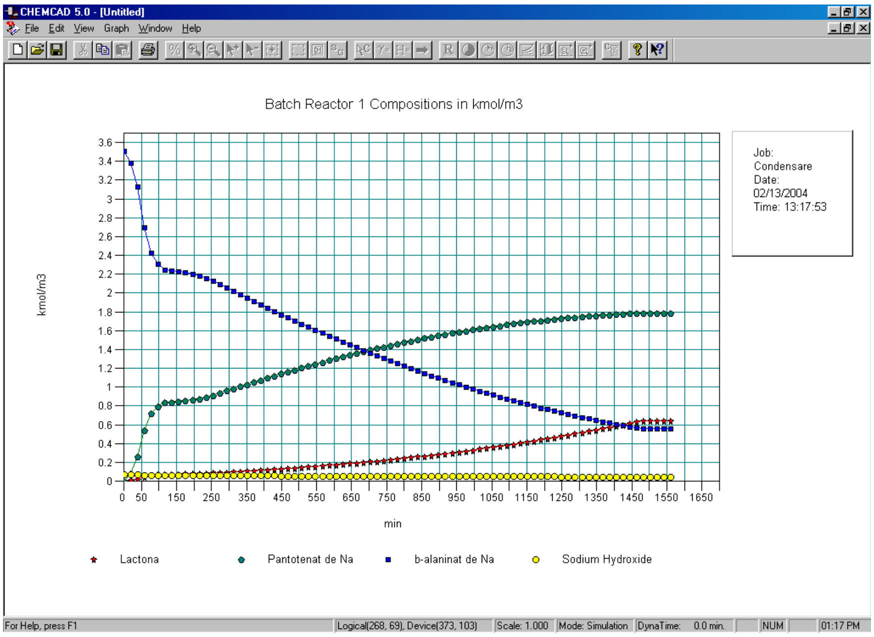


Figure 2. Chemical species concentrations variation during the synthesis process

The variation of the temperatures (reactor solution and jacket cooling agent) in case of using one PID controller for the reactor temperature, are presented in figure 3.

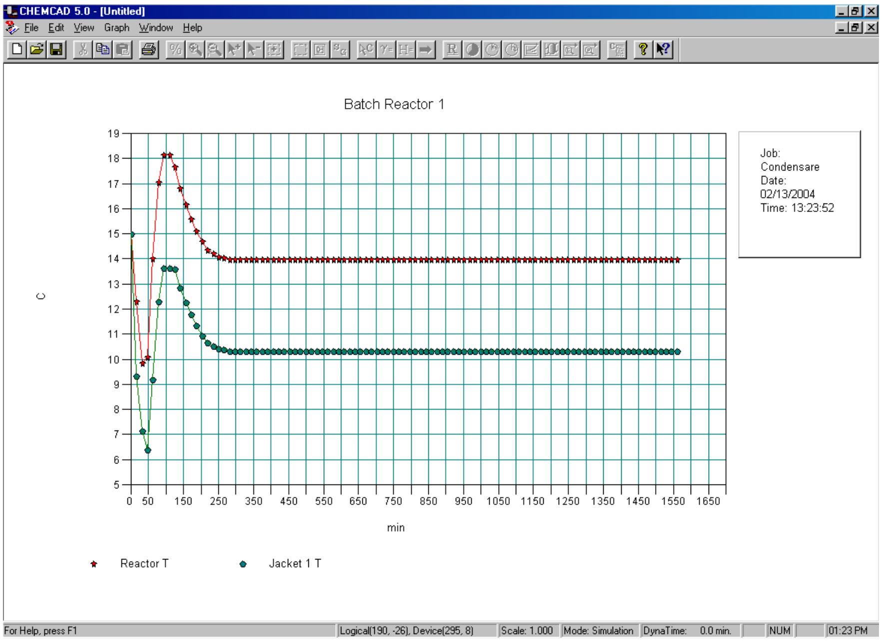


Figure 3. Temperatures variation during the synthesis process (with one PID controller)

From the figure 3 one can observe that the reactor solution temperature during sodium pantothenate synthesis is good controlled between 13 and 15^{o}C (set point temperature of the PID controller is 14^{o}C).

In the industrial plant, temperature control system for the reactor mass is not used [2]. This fact leads to a poor temperature control for the reactor solution and to a cooling agent consumption greater than the situation when a temperature control system is used.

The variation of the temperatures (solution from the reactor and jacket cooling agent) in case of using no temperature control system for the reactor temperature, are presented in figure 4.

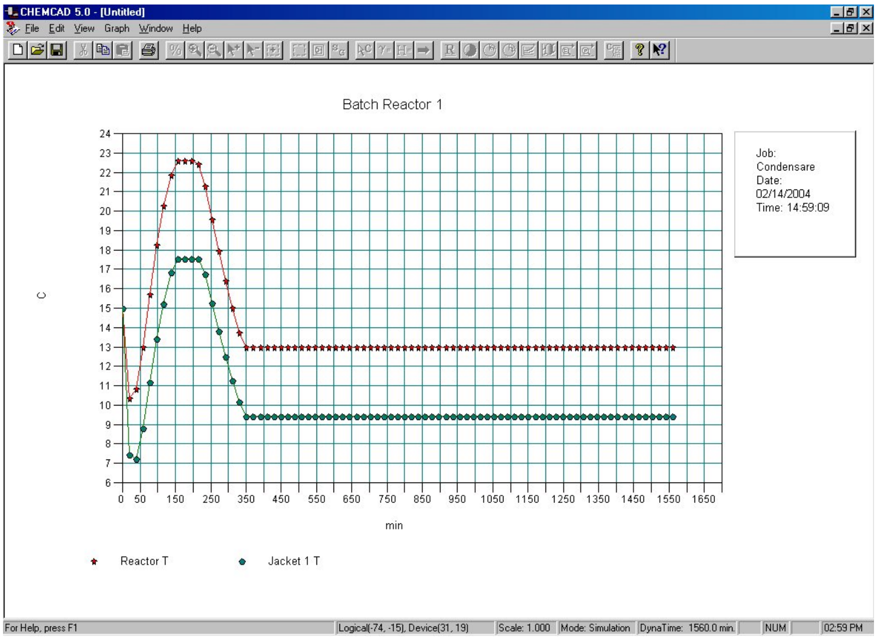


Figure 4. Temperatures variation during the synthesis process (without PID controller)

Comparing the results of the process simulation with one temperature control system, using pantolactone solution flow as manipulated variable, and the simulation results obtained using no control system for reactor temperature, one can observe that the introduction of the temperature control system leads to a better reactor temperature control.

The results of mathematical modeling and simulation for sodium pantothenate synthesis show the fact that introduction of one reactor temperature control system (using pantolactone flow added into the reactor or cooling agent flow from the reactor jacket) leads to a large cooling agent economy (10 – 15 %).

The annual cooling agent economy for sodium pantothenate synthesis in case of using a reactor temperature control system is $6,000.

The value of annual cooling agent economy was calculated considering the number of annual batches, the heat-calculated values for a batch (with and without reactor temperature control system) and the price of the cooling agent [7].

At the same time, introduction of one reactor temperature control system, using pantolactone flow or cooling agent flow, leads to a better reactor temperature control, with benefic consequences on the quality of the product.

4. CONCLUSIONS

In this paper the discontinuous synthesis of sodium pantothenate has been described. The synthesis process was modeled and simulated using ChemCAD 5.0 software package.

The sodium pantothenate synthesis process was modeled and simulated in two different situations. The first situation considers a control of the reactor temperature using a PID controller (pantolactone solution flow as manipulated variables) and in the second situation no reactor temperature control system is used.

The variations of different parameters (concentration of chemical species from the reactor solution, reactor solution temperature and cooling agent temperature) during the sodium pantothenate synthesis were presented.

A control system for the reactor temperature leads to a large cooling agent economy ($6,000 per year) and also, to a better reactor temperature control, with benefic consequences on the quality of the product.

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

5. REFERENCES

1. G. Neamțu, [1996], Substanțe naturale biologic active, Editura Ceres, București, vol. 1, pag. 329 – 346.
2. ***, [2001], Regulament de fabricație „Pantotenat de calciu", S.C. Terapia S.A., Cluj-Napoca, Romania
3. C. Cormos, S. Agachi, [2000], Modeling and simulation the process of synthesis of D,L calcium pantothenate, International Conference on Quality Control, Automation and Robotics Q&A-R 2000, Cluj-Napoca, vol. 2, pag. 7 – 12.
4. C. Cormos, S. Agachi, [2000], Modelling and simulation the synthesis process of sodium pantothenate, International Symposium of Chemical Engineering - SICHEM 2000, Bucharest, Romania, pag. 305 – 312
5. C. Cormos, S. Agachi, [2002], Modeling and simulation of sodium beta-alaninate synthesis using ChemCAD and HYSYS Plant software packages, International Conference on Automation, Quality and Testing, Robotics A&QT-R 2002 (THETA 13), Cluj-Napoca, Romania
6. C. Cormos, S. Agachi, [2003], Modeling and simulation of pantolactone synthesis using ChemCAD, 30-th International Conference of Slovak Society of Chemical Engineering, Tatranske Matliare, Slovakia
7. C. Cormoş, [2004], Modelarea matematică şi simularea sintezei pantotenatului de calciu racemic, Teză de doctorat, Cluj-Napoca, pag. 203 – 214