STUDIA UNIVERSITATIS BABES-BOLYAI, CHEMIA, XLIX, 2, 2004

Dedicated to Professor Valer Fărcăşan at his 85th anniversary

MODELING AND SIMULATION OF RESIDUAL PANTOLACTONE EXTRACTION FROM CALCIUM PANTOTHENATE SOLUTION

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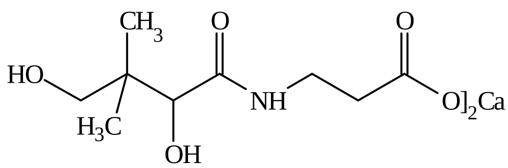
ABSTRACT. In this paper the mathematical model and the simulation for the extraction process of residual pantolactone from racemic calcium pantothenate solution have been described. The aqueous solution of calcium pantothenate resulted from synthesis process contains residual racemic pantolactone that is extracted using dichloromethane. The pantolactone extraction process can be done in two technological ways. The first possibility is to use an extraction system consisting of a reactor and a packed extraction column, operated batchwise. The second possibility is to use a continuous counter-current centrifugal extractor. In this second way, economy of time, extraction solvent and energy savings are achieved. The mathematical models of the extraction process were simulated using ChemCAD 5.0 software package. From the simulation results very valuable information can be obtained regarding real plant operation.

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, 6] (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 including chemical steps and physical separations of the intermediaries and the final product. 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 these processes were to find the best operating points for the equipment, to try different control algorithms, to improve the energy consumption of the plant [4, 5, 6].

In this paper the mathematical model for the extraction process of residual pantolactone from racemic calcium pantothenate solution using dichloromethane has been described. The extraction of residual pantolactone from racemic calcium pantothenate solution is done in order to purify the finite product [2].

The pantolactone extraction process from the calcium pantothenate aqueous solution is achieved using dichloromethane as extraction solvent [3].

Practically, pantolactone extraction process can be performed using two technological ways. The first possibility is to use an extraction system consisting of a reactor and a packed extraction column, operated batchwise. This technological way for pantolactone extraction is used in the real plant [2]. Dichloromethane is loaded in the reactor and racemic calcium pantothenate aqueous solution is loaded in the extraction column. Dichloromethane from the reactor is vaporized and, after condensation and cooling in two heat exchangers, enters in the extraction column. Pantolactone from the aqueous solution is extracted by dichloromethane and, because of the density difference, the organic phase (pantolactone in dichloromethane) leaves the extraction column and returns in the reactor.

The second possibility is to use a continuous counter-current centrifugal extractor. In this second way, economy of time, extraction solvent and energy savings (it is not necessary to make the vaporization – condensation cycle for pantolactone extraction) are achieved.

2. MODELING AND SIMULATION OF THE EXTRACTION

The extraction process of residual pantolactone from calcium pantothenate solution was modeled and simulated using ChemCAD 5.0 software package.

The parameters of the mathematical models for racemic pantolactone extraction are presented in tables 1, 2 and 3 [2, 6].

Table 1.

Extraction reactor characteristics

Reactor volume	4 m^3
Jacket volume	0.4 m^3
Heat transfer area	10 m^2
Reactor diameter	1.6 m
Impeller diameter	1 m
Impeller speed	180 rpm
Motor power	5 kW

Table 2.

Packed column characteristics

Column volume	6 m^3
Number of stages	6
Packing characteristics	Raschig ring D x H x d = 25 x 30 x 15 mm

Table 3.

Centrifugal extractor characteristics

Number of stages	6
Phases circulation mode	Counter-current

Pantolactone extraction coefficient in dichloromethane – water system [3]:

$$K = \frac{X_{Pantolactone\ in\ dichloromethane\ phase}}{X_{Pantolactone\ in\ water\ phase}} = 2$$

The two technological ways for residual pantolactone extraction process were modeled and simulated with ChemCAD 5.0 software package.

Figure 1 presents the main window of pantolactone extraction application developed using ChemCAD 5.0 software packages for the mathematical modeling and the simulation of extraction process using a continuous counter-current centrifugal extractor.

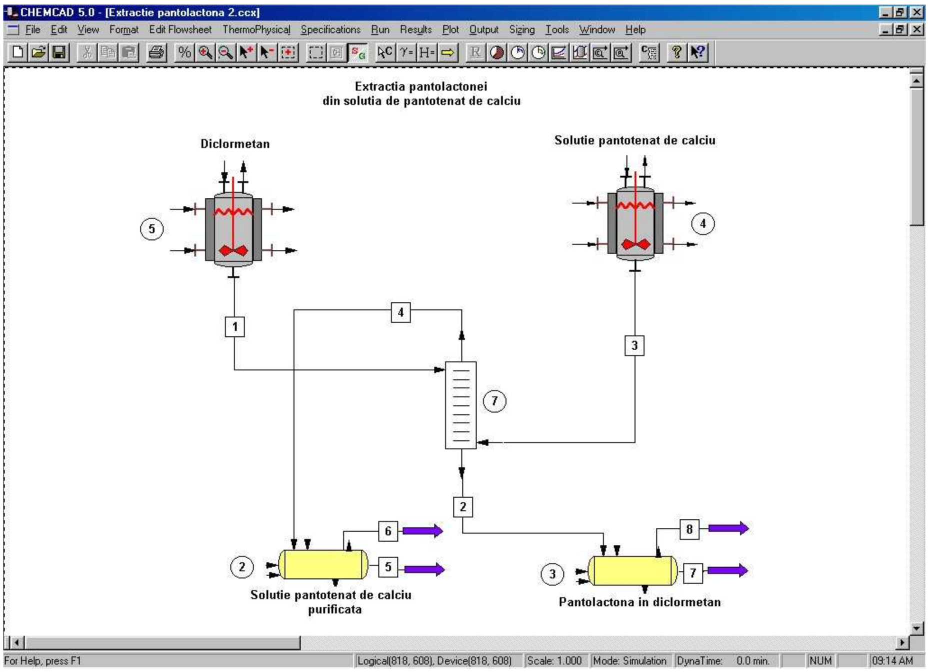


Figure 1. Simulation of pantolactone extraction using a centrifugal extractor

Figure 2 shows the main window for pantolactone extraction application (developed in ChemCAD 5.0) using a reactor and a packed column.

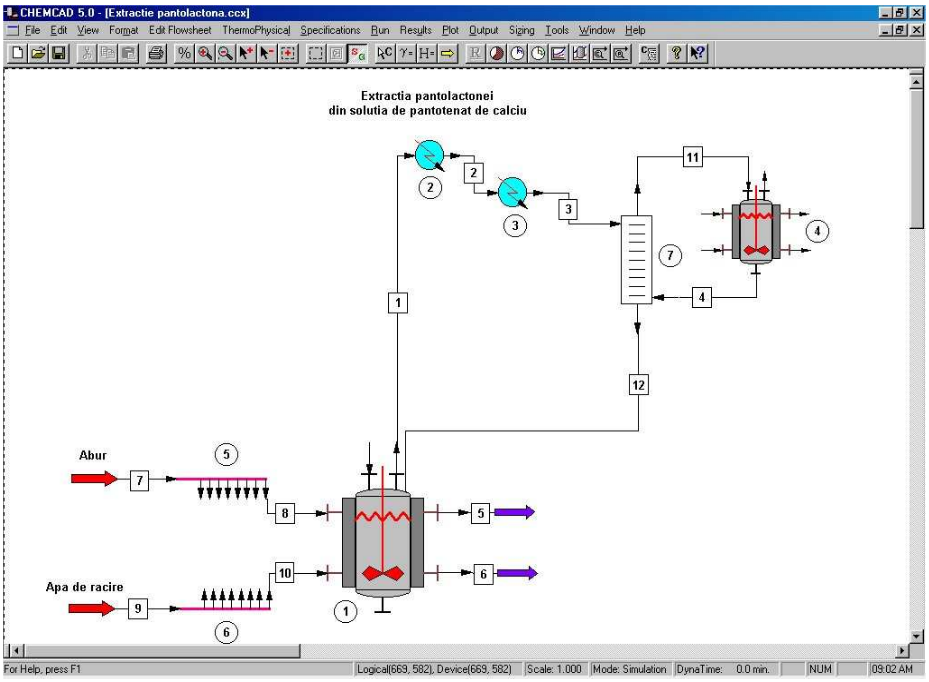


Figure 2. Simulation of pantolactone extraction using a packed column

3. RESULTS AND DISCUSSIONS

The mathematical model of residual pantolactone extraction process from calcium pantothenate solution was simulated using ChemCAD software package.

For extraction process using a counter-current centrifugal extractor, the variation of components quantities for the aqueous phase (calcium pantothenate solution) leaving the centrifugal extractor are presented in figure 3.

The variation of composition (mass fractions) for the aqueous phase (racemic calcium pantothenate solution) that leaves the centrifugal extractor is presented in figure 4.

The variation of the composition (mass fractions) for the organic phase (pantolactone in dichloromethane) that leaves the centrifugal extractor is presented in figure 5.

For the extraction process using a reactor and a packed column, the variation of chemical species composition (mass fractions) for the solution collected in reactor during the extraction process are presented in figure 6.

The variation of the composition (mass fractions) for the aqueous solution from the extraction column during the process is presented in figure 7.

The variation of the composition (mass fractions) for the flow that leaves the extraction column and goes to reactor is presented in figure 8.

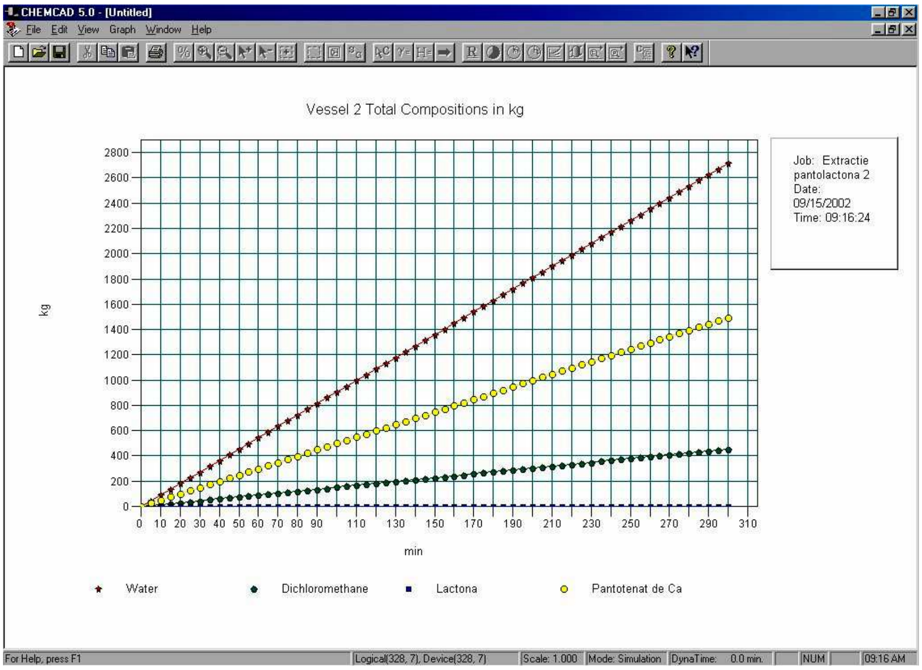


Figure 3. Variation of chemical species quantities for the aqueous phase

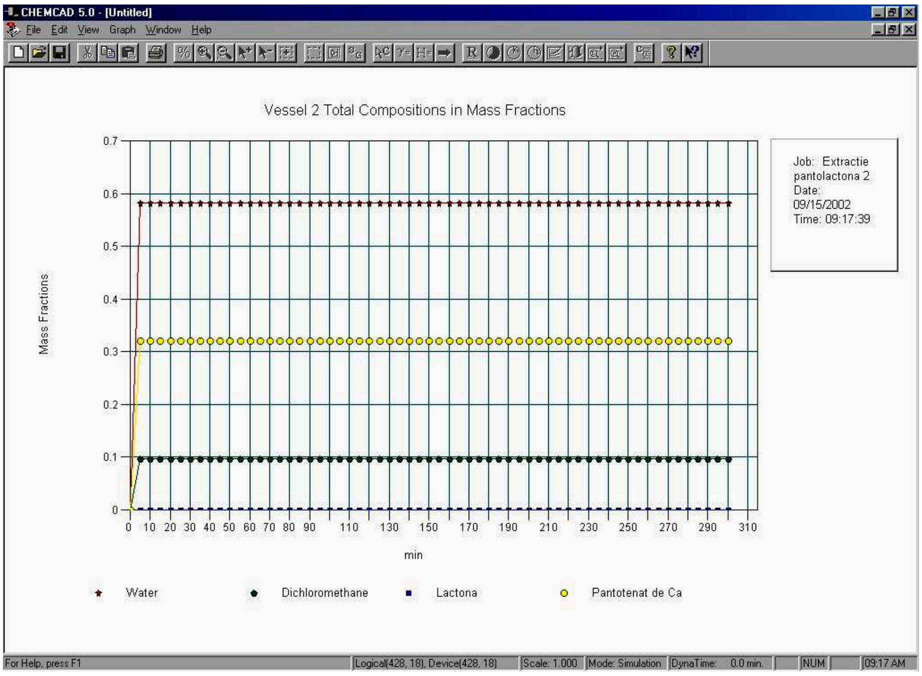


Figure 4. Variation of composition for the aqueous phase (mass fractions)

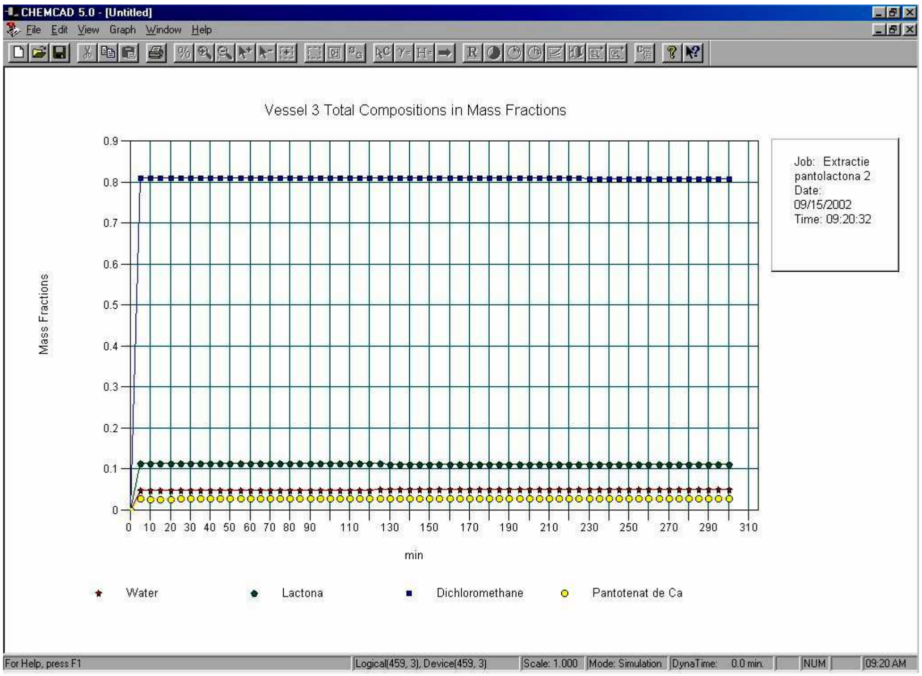


Figure 5. Variation of composition for the organic phase (mass fractions)

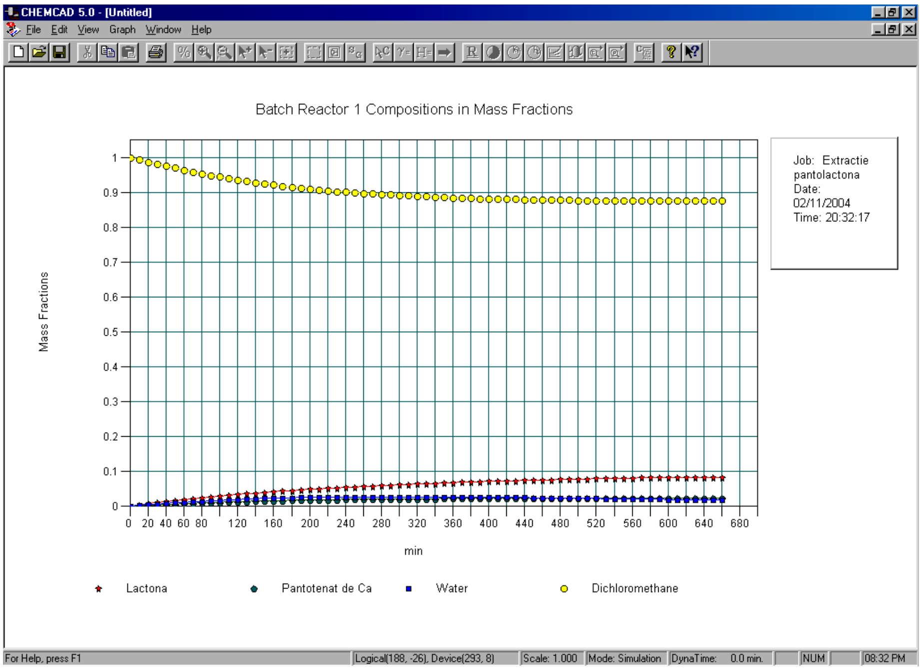


Figure 6. Variation of composition for the organic phase from the reactor

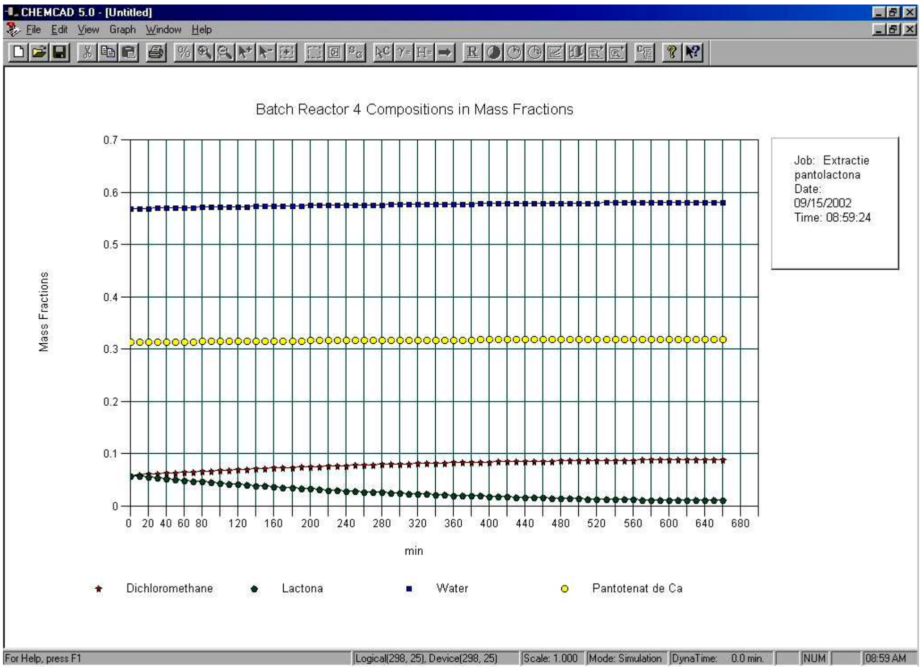


Figure 7. Variation of composition for the aqueous phase from the extraction column

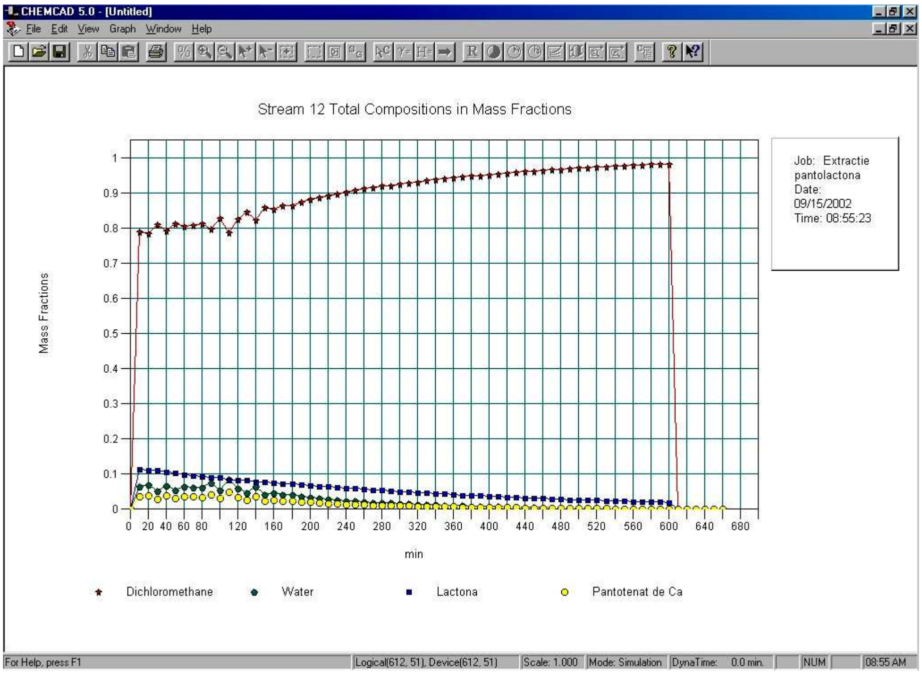


Figure 8. Variation of the composition for the flow that leaves the extraction column

The main difference between the first and the second way of pantolactone extraction is the utility consumption. Utility consumption is greater when we use an extraction system composed of a reactor and a packed column [6].

In the table 4, the utility consumptions and extraction time for one racemic calcium pantothenate batch are presented.

Table 4.

Utility consumption and extraction time for pantolactone extraction process

Comparison criterion	Reactor and packed column	Centrifugal extractor
Utility consumption (for one calcium pantothenate batch)	Steam (R 1): 0.5333 Gcal Cooling water (R 1): 0.0634 Gcal Cooling water (SC 2): 0.3283 Gcal Refrig. agent (SC 3): 0.0157 Gcal Electric power (R 1): 50 kWh	Electric power: 20 kWh
Extraction time	10 h	5 h

Considering the value of technologic utilities for the extraction system with reactor and packed column ($18,700/year) and adding the dichloromethane losses ($18,300/year) results as evident the attractiveness of the extraction system that uses a counter-current centrifugal extractor [2, 6].

When we use a counter-current centrifugal extractor, the annual economy is $37,000 (counting only the utilities consumption and the dichloromethane losses).

In addition to the above-mentioned aspects, operating a counter-current centrifugal extractor is much easier and the environmental impact is lower than using an extraction system with reactor and packed column operated batchwise [6].

4. CONCLUSIONS

In this paper the extraction process of residual pantolactone from racemic calcium pantothenate solution was presented. Two technological ways for residual pantolactone extraction were considered for analysis. The first possibility is to use an extraction system consisting of a reactor and a packed extraction column, operated batchwise. The second possibility is to use a continuous counter-current centrifugal extractor.

The mathematical models of the pantolactone extraction process were simulated using ChemCAD 5.0 software package. The variations of different parameters during the extraction process were presented.

The mathematical models proved to be a reliable tool for analyzing pantolactone extraction process. Using the mathematical models of the extraction process and the simulation results, the two technological ways of residual pantolactone extraction process were analyzed.

It was demonstrated, by simulation results, that using a centrifugal extractor the annual economy is $37,000 (counting only the utilities consumption and dichloromethane losses). Also, operating a centrifugal extractor is much easier and the environmental impact is lower compared to the situation of using an extraction system with reactor and packed column.

In conclusion, using a counter-current centrifugal extractor, economy of time, extraction solvent and energy savings (it is not necessary to make the vaporization – condensation cycle for pantolactone extraction) are achieved.

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