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Simulation of Safe Processes Using Aspen Plus: an Economic Evaluation

Araya Ajchariyapagorn[1], Supaporn Douglas[1*], Peter L. Douglas[2], and Suwassa Pongamphai[1]

[1]*Department of Chemical Engineering, King Mongkut's University of Technology Thonburi, Bangkok 10330, Thailand.*
[2]*Department of Chemical Engineering, University of Waterloo, Canada.*

Abstract

A continuous process for the extraction of nimbin from neem seeds using supercritical CO_2 was simulated using the AspenPlus™ simulation system. A mathematical model was built to simulate the extraction process and experimental data (Tonthubthimthong et al., 2001) were used to validate the model. The mathematical model of the complete process was coded in AspenPlus. Process simulation and optimisation, to minimise energy consumption, was carried out. Simulation and optimisation results are presented.

Keywords: Nimbin, Neem, Simulation, Supercritical Fluid, Extraction

1.0 Introduction

$C_{30}H_{36}O_9$ is a medical substance which can be extracted from neem seeds. Commercial processes for the production of nimbin use supercritical carbon dioxide. This work builds on the results of projects currently underway in the Department of Chemical Engineering at KMUTT in which models, validated by experiments of nimbin extraction using supercritical CO_2, were developed. Aspen Plus was used to develop a simulation of the CO_2 extraction unit and the balance of plant including compressors and separators. Supercritical extraction models are not currently available in Aspen Plus. The existing modules within Aspen Plus were used along with the modeling results from Tonthubthimthong et al. (2002) and Mongkholkhojornsilp et. al. (2005) to develop an overall simulation of the process.

2.0 Simulation of supercritical CO_2 extraction using Aspen Plus

2.1 Model development

Simulation of the supercritical CO_2 extraction process (Figure 1) was performed using Aspen Plus. Aspen Plus is a chemical process simulation tool used in both research and industrial applications. Aspen Plus has built-in process models for common types of process units including reactor, heat exchanger, compressors and separators. Aspen Plus has a variety of different physical property models available to simulate a variety of chemical systems.

* *Corresponding author: Tel.: +1-519-888-4601; Fax: +1-519-888-5365; Email: pdouglas@cape.uwaterloo.ca*

Physical properties

In our work, Lee-Kesler-Plocker model and group contribution method (for nimbin properties) will be applied.

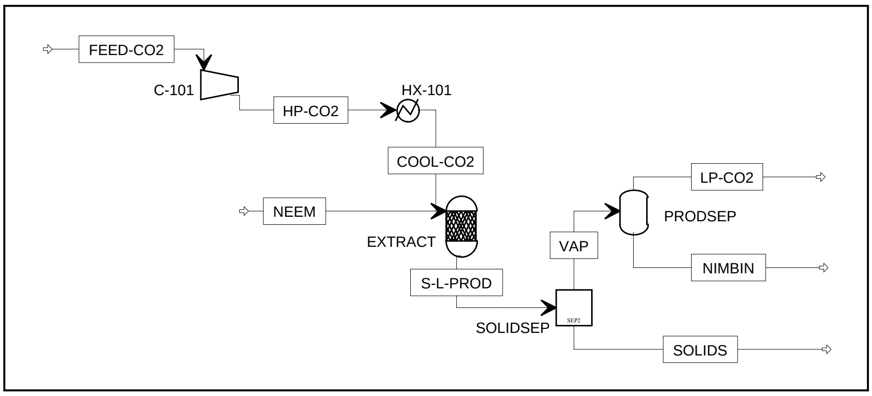

Figure 1 Process flow sheet of nimbin extraction (reference case)

Compressor and Heat exchanger

Compressor is assumed to operate with a polytropic using ASME method. Heat exchanger was assumed that no pressure drop occurred. The initial set up for operating pressure in compressor and temperature in heat exchanger are 20 MPa and 308 K respectively. The both values will be changed with optimization loop.

Extractor

Aspen Plus does not contain a unit operator model for supercritical extraction, thus a stoichiometric reactor was use in this work. The reactor was used to provide yield from regression analysis as a conversion of equation below:

$$a\ \text{Neem} + b\ CO_2 \rightarrow Y\ \text{NIMBIN}$$

Separators

The complete separation between the solid and gaseous components at the exit was assumed to occur and the second separator was set to 300 K for separating liquid nimbin from CO_2.

2.2 Optimisation and Economic Evaluation

The optimisation in this feasibility study is to build a nimbin plant. The plant has the capacity to produce about 1,600 kilogram per year of nimbin by the extraction of neem with supercritical carbon dioxide.

The options analyzed in this section include 2 cases are:

- Reference case (Figure 1)
- Recycle case (Figure 2)

The optimizing Model:

The objective function $\rightarrow$ to minimize energy

ENERGY = Energy required in (compressor unit + heat exchanger unit)

Equality constraint → Nimbin product = 0.2 kg/hr
Inequality constraint → Fraction yield ≤ 1

The method for doing optimization used is SQP (Sequential Quadratic Programming).

For economic evaluation, Aspen Plus-nimbin extraction has built a techno-economic model of the “reference case” and “recycle case” to help evaluation of the feasibility of the project. The “reference case" is the real plant that has vent CO_2 after product separation. And the “recycle case” is the reduce cost that has recycle carbon dioxide after separating from the product.

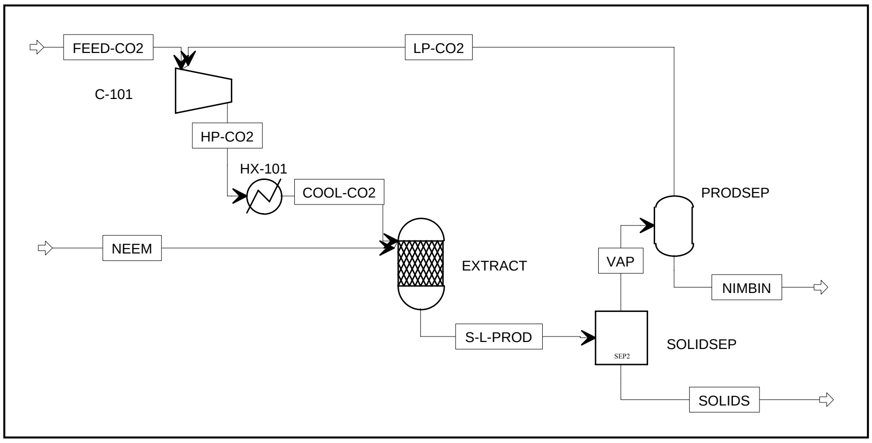

Figure 2 Process flow sheet of nimbin extraction (recycle case)

The techno-economic model simulates continued operation of the plant for the base year (year 0 = 2004). It is assumed that the plant is commissioned at the end of project year 1 (2005).

The model builds up costs based on reference prices. The input prices of raw materials to the plant were agreed with the company. Price and cost forecasts are based on Sinnott (1996) and Bravi (2002).

Variable and fixed costs of production are built up from yield factors; plant operating requirements and forecast prices and costs for a fifteen years operating life (from project year 1 to project year 15).

3.0 Simulation Results

This section is a simulation result from complete model of 2 cases: “reference case” and “recycle case”, Table 1 shows the operating condition and simulation results of 2 cases. The optimization results with minimization of energy requirement shows in Table 2. For a reference case operating at 27.4 MPa, a unit nimbin production cost of 835 $/kg was found. Recycle CO_2 case the unit nimbin production cost was found to be 777 $/kg at 27.2 MPa. This clearly shows that a recycle case with an operating pressure of 27.2 MPa features the lowest unit nimbin production cost. The annual rate diagram for two cases is plotted in figure 3.

Although the presented results suggest that SFE-extracted nimbin with recycle CO_2 has a market future, further information should be gathered concerning the transport phenomena at varying operating conditions and the profile of nimbin quality during the extraction.

Table 1 Operating conditions and simulation results

Operating condition	**Reference case**	**Recycle CO_2**
Tempearature (K)	308	308
Pressure (MPa)	27.4	27.2
Carbon dioxide flowrate (l/min)	57	0.43
Neem flowrate (kg/hr)	1,093	1,112
Nimbin flowrate (kg/hr)	0.2	0.2

Table 2 Optimization results

Operating cost and profitability of SCFE plant (year 15, values in USD)		
Item	**Reference case**	**Recycle CO_2**
Revenue ($/yr)		
Nimbin sale	1,920,000.00	1,920,000.00
Costs ($/yr)		
Annual capital cost	282,384.45	268,301.44
Fixed operating cost	553,830.80	523,045.32
Variable cost	773,975.01	712,480.72
Miscellaneous material	7,669.80	7,304.45
Total	1,617,860.05	1,511,131.94
Annual production cost	**835**	**777**
Net value ($/yr)	302,139.95	408,868.06
Internal return rate (IRR)%	**16.43**	**25.163**

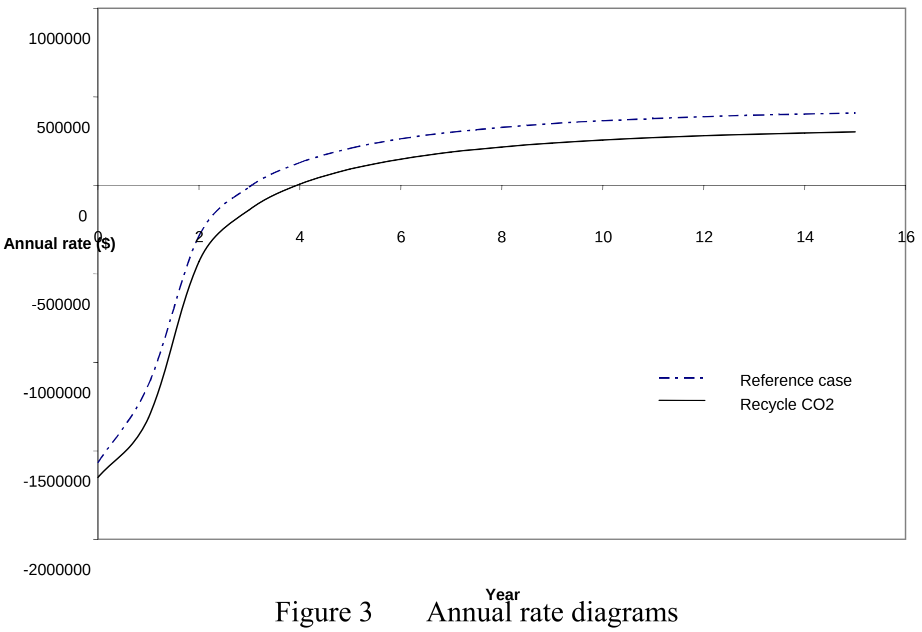

Figure 3 Annual rate diagrams

4.0 Conclusions

In order to design and operating whether Supercritical CO_2 offers a better technique to extract nimbin from neem seeds a parametric process layout was devised and a mathematical model-regression analysis of it was built. The simulation of the behavior of the modeled nimbin extraction plant with reference case and recycle case was carried out and the process operation was optimized-minimising energy or power consumption on both of them. The results of the optimisation yielded the optimal values of the operating conditions and the optimal operating schedule for a given flowrate of supercritical CO_2 for the proposed parametric process set-up, a recycle CO_2 case, is mot profitable. The operating condition is the pressure in the extractor vessel which was calculated to be 27.2 MPa. Correspondingly, the production cost estimated to be 777 $/kg, a figure that, although high, is still acceptable for a product destined to the ever-glowing market of high-quality food product.

Acknowledgement

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