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Application of Genetic Algorithm on Model-Based Optimisation of Supercritical Carbon Dioxide Extraction: An Overview

Mohd Amzar Mohamed Zahari[a,b], Liza Md. Salleh*[,a,b]

[a]Department of Bioprocess Engineering, Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81310, Skudai, Johor, Malaysia.
[b]Centre of Lipid Engineering Applied Research (CLEAR), Ibnu Sina Institute, Universiti Teknologi Malaysia, 81310, Skudai, Johor, Malaysia.
i.liza@cheme.utm.my

Green supercritical carbon dioxide extraction technology has gained enormous interest especially in the application of extraction of natural products. The use of carbon dioxide as solvent in the extraction process is very advantageous as carbon dioxide is cheap, non-toxic, high selectivity, and can easily be separated. Supercritical carbon dioxide extraction is considered as a complex process as more factors affect the outcome of the process as compared to conventional extraction methods. This technology requires higher cost to setup and maintain the equipment. For these reasons, the whole process needs to be fully understood to ensure that the process is well optimised. Mathematical modelling is a way to explain the relationship between process variables and the outcome of the process. The optimisation of supercritical carbon dioxide extraction needs to be highly integrated to be feasible, which means that a complex mathematical model is involved. In overcoming this problem, genetic algorithm was applied in several studies. Genetic algorithm is one of the optimisation methods that is able to optimise a complex and large scale of problems, with high accuracy and practicality. This paper intends to give an overview on the application of genetic algorithm in the optimisation of mathematical modelling of supercritical carbon dioxide extraction process.

1. Introduction

Supercritical carbon dioxide extraction is one of the green technologies in extraction processes. Carbon dioxide favourable to be used as solvent in this extraction method due to its lower critical temperature and critical pressure (304.12 K and 73.7 bar). Carbon dioxide is also cheap, easily obtained, non-hazardous because it is highly inert, and easily separated from the extract (Thana et al., 2008). The use of carbon dioxide will also ensure the good quality of the extract because carbon dioxide is highly selective and its low critical temperature preserves the thermolabile bioactive compounds from degradation (Piras et al., 2009).

Supercritical carbon dioxide extraction manipulates the characteristic of carbon dioxide in its supercritical state. Supercritical state is a phase where the density of the liquid phase diminishes and the vapor density increases due to the higher vapour pressure. At this phase, the liquid and the vapour state are no longer able to be differentiated. A solvent in supercritical state can effuse through solid matrix like a gas and dissolve the solute like a liquid. The physical characteristic of the supercritical carbon dioxide, which is in between gas and liquid, makes the process highly tunable to favour the process. The parameter of supercritical carbon dioxide can be adjusted to change its behaviour and physicochemical properties into more gas-like or liquid-like.

The operating pressure and temperature of a supercritical carbon dioxide extraction system are highly correlated with the density of the carbon dioxide. Carbon dioxide density is favoured to be as high as possible in order to achieve the maximum solubility and solvent power. Other than temperature and pressure; carbon dioxide flow rate, introduction of entrainer, and particle size of the sample are also affecting the outcome of the supercritical carbon dioxide extraction process.

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In the extraction of natural products, supercritical carbon dioxide extraction have been applied for the extraction of a wide range of beneficial plant species such as Moringa oleifera (Zhao and Zhang, 2013), Pinus pinea (Salgin and Salgin, 2013), Strobilanthes crispus (Liza et al., 2010), Mangifera indica leaves (Dos Santos et al., 2013), Cannabis sativa (Tomita et al., 2013), grape seed (Duba and Fiori, 2015), coffee beans (Hasan and Farouk, 2013), nutmeg oil (Machmudah et al., 2006), Posidonia oceanic (Pilavtepe and Yesil-Celiktas, 2013), Chamomilla recutita (Rahimi et al., 2011), neem seeds (Zahedi et al., 2010), and Eugenia caryophillus (Hatami et al., 2010).

2. Mathematical Modelling of the Process

Supercritical carbon dioxide extraction is a complex process with various interactions of affecting factors and lack of comprehensive fluid dynamic knowledge of supercritical fluid in the extraction process. The number of factors affecting the process is more than conventional extraction methods. The supercritical fluid extraction can be affected by the tuneable operating parameters such as temperature, pressure, flow rate, and other extrinsic factors such as sample characteristic, the interaction with the desired organic compounds and many environmental factors (Sharif et al., 2014). Therefore, a mathematical model is used to describe the process as it reflects the physical behaviour of the solid structure and experimental observations.

Process modelling of supercritical fluid extraction is usually employed to correlate the experimental data with theoretical explanations. The main objective of the process modelling of supercritical fluid extraction is to define the parameter for process design, such as equipment dimensions, operating pressure and temperature, solvent flow rate and particle size of the sample. These parameters are used as a simulation tool to predict the overall extraction curve (OEC) of supercritical fluid extraction in order to estimate the process viability in industrial scale (Mezzomo et al., 2009). The most common mathematical models applied in supercritical carbon dioxide extraction are equilibrium solubility-based model and kinetic mechanism-based model.

Equilibrium solubility-based model is a density-based model, which correlate the solubility of a pure solute with temperature, pressure, and density of a pure supercritical solvent. This mathematical correlation model is widely used because of its simple application. Solubility models avoid the use of physicochemical properties as in thermodynamic models, which are difficult to determine experimentally and need to be estimated by various methods (Keshmiri et al., 2014). There are numerous solubility models that have been introduced and successfully applied in the supercritical carbon dioxide extraction, and some of the most widely used solubility models are Chrastil model (Chrastil, 1982), Mendez-Santiago and Teja model (Mendez-Santiago and Teja, 2000), and Gordillo model (Gordillo, 1999).

Kinetic mechanism-based model is developed from the mass transfer mechanism of the extraction process. The kinetic models are differentiated by the theory used in the mechanism of the mass transfer. Basically, all mass transfer mechanism is the diffusion process of solute from solid internal into solid surface and dissolution of solute from the solid surface to the supercritical solvent. There are several models describing the mechanism of mass transfer in the supercritical fluid extraction such as the Shrinking core model (Goto et al., 1996), the Broken and intact cell model (Sovová, 2005), and the Broken and intact plus shrinking core model (Fiori et al., 2009).

3. Application of Genetic Algorithm in Process Optimisation

Process optimisation of supercritical carbon dioxide extraction is highly essential, especially for the purpose of up-scaling the process, as setting up a supercritical carbon dioxide extraction unit requires large investment, operation and maintenance costs. As the optimisation of the process need to be highly integrated to be economically viable, kinetic mechanism-based model is selected to present the correlation of the affecting factors and the outcome of the process. The optimisation of the supercritical carbon dioxide process by using its best fitted kinetic mechanism-based model can be done by genetic algorithm (Hatami et al., 2010).

Genetic algorithm is the first and can be considered as the father of all evolutionary algorithms. Evolutionary algorithms are stochastic search methods that mimic the metaphor of natural biological evolution and/or the social behaviour of a species, which is guided by learning, adaptation, and evolution. Genetic algorithm was developed by Holland (1975) based on the Darwinian principle of the 'survival of the fittest' and the natural process of evolution through reproduction. In general, the fittest individuals of any population tend to reproduce and survive to the next generation. However, inferior individuals can, by chance, survive and also reproduce.

Genetic algorithm has been shown to solve linear and nonlinear problems by exploring all regions of the state space and exponentially exploiting promising areas through mutation, crossover, and selection operations applied to individuals in the population. Based on its demonstrated ability to reach near-optimum solutions to large problems, the Genetic algorithm method has been used in many applications in science and engineering. Genetic algorithm has been applied in the area of supercritical carbon dioxide extraction to obtain the value of adjustable parameters in mathematical models and to find the optimal value of process parameters. In this overview, we only focus on the application of genetic algorithm for the optimisation of process parameters of supercritical carbon dioxide extraction. The process flow chart of this optimisation process is as in Figure 1. Kinetic mechanism-based model is used as the fitness function.

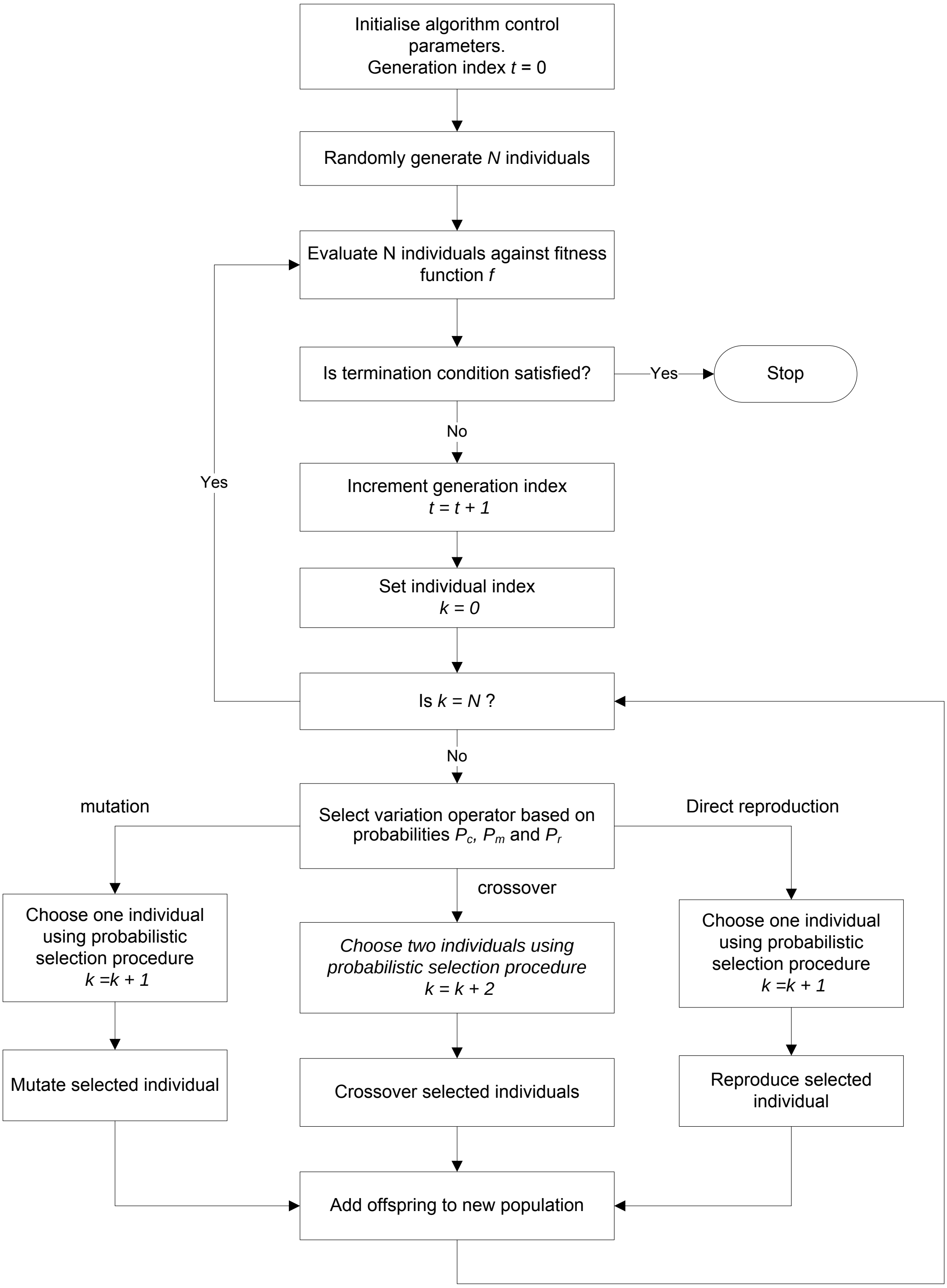

Figure 1: Process flow chart of genetic algorithm (Zahedi et al., 2010)

Genetic algorithm starts with a population of random members or regimes. A new member, referred to as offspring, is generated from one or two randomly chosen parents. The offspring generated is added to the population pool in the reproduction step. Next, two members are taken at random out of the pool. Among these two members, the less optimal is removed from the population. This “survival of the fittest” elimination process ensures that the population’s general fitness keeps increasing. The elimination process is repeated until a satisfactory regime is acquired among the existing population, or until no further improvement has been obtained for a pre-specified number of generations.

Genetic algorithm finds the optimum value by evaluating each possible solution according to the fitness value calculated by the fitness function. The process is iterative and each iteration is called as generation. In each generation, every possible solution is evaluated and the more fit solution is stochastically selected to form the new generation. An example of how genetic algorithm works in finding the optimum process parameter value of the supercritical carbon dioxide extraction is shown in Figure 2, obtained in a study by Bashipour and Ghoreishi (2012). We can see the variation of fitness value over generation produced by genetic algorithm in finding the optimal operating parameters (pressure, temperature, and flow rate of carbon dioxide) for the extraction of β-Carotene from Aloe barbadensis Miller. The optimisation process is terminated at generation 50 as it is clear that this generation’s number was enough to reach an accurate optimisation.

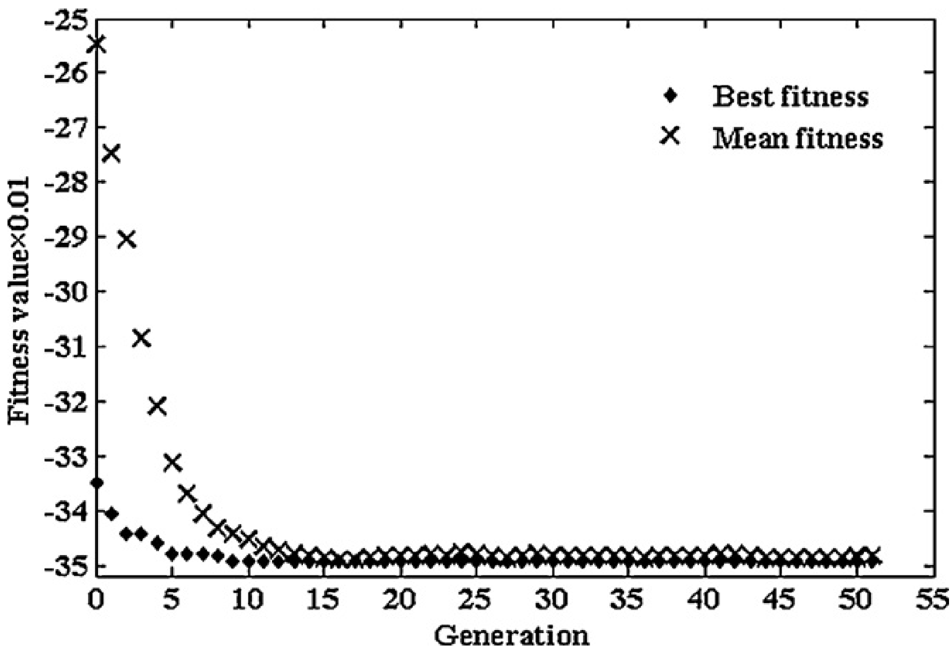

Figure 2: Variation of fitness function versus generation at L = 12.5 cm, ID = 0.9 cm, Rp = 0.3 mm and dynamic time = 260 min (Bashipour and Ghoreishi, 2012)

Several studies on the application of genetic algorithm in process optimisation of supercritical carbon dioxide extraction have been published. Those studies are the extraction of clove oil (Hatami et al., 2010), nimbin from neem seeds (Zahedi et al., 2010), chamomile (Rahimi et al., 2011), St. John's Wort (Hatami et al., 2012), and β-Carotene from Aloe barbadensis Miller (Bashipour and Ghoreishi, 2012). Those literatures are summarised in Table 1.

In those studies, genetic algorithm is used to determine the distribution coefficient, the equilibrium constant, and also to find the optimum supercritical carbon dioxide extraction process parameters in order to maximise the extraction yield, number of extraction, and profit. Zahedi et al. (2010), in his study, compared the ability of genetic algorithm technique with the traditional Gradient Search optimisation technique in optimising the supercritical carbon dioxide extraction. He concluded that genetic algorithm method is much more efficient, in terms of computational effort in reaching the optimal conditions.

Table 1: Application of genetic algorithm on process optimisation in previous studies

Author	Purpose of Application	Result
Zahedi et al. (2010)	Profit optimisation of supercritical carbon dioxide extraction of nimbin from neem seeds.	Optimal process parameters to achieve maximum profit are 305 K, 200 bar, 0.967 cm^3/min, and 0.1431 cm neem particle diameter.
Hatami et al. (2010)	Oil yield optimisation of supercritical carbon dioxide extraction of clove buds.	Maximum clove oil extraction is achieved at 10 MPa and 304.2 K.
Rahimi et al. (2011)	To determine the distribution coefficient of chamomile extract between solid and solvent. Optimisation of chamomile extraction yield.	Optimum chamomile extraction yield is obtained at 313.15 K and 20 MPa.
Hatami et al. (2012)	To determine the equilibrium constant of St. John's Wort extract between solid and fluid phase. Optimisation of extraction yield of supercritical carbon dioxide extraction of St. John's Wort.	Optimum extraction yield is obtained at 313 K and 20 MPa.
Bashipour and Ghoreshi (2012)	Yield optimisation of supercritical carbon dioxide extraction of β-Carotene from Aloe barbadensis Miller.	Highest yield of β-Carotene (0.3524 g β-Carotene/kg dry sample) is obtained at 333.15 K, 29 MPa, and 1 mL/min carbon dioxide flow rate.

4. Conclusion

Genetic algorithm is one of the promising optimisation method for the supercritical carbon dioxide extraction process. It is able to solve complex and highly integrated kinetic mechanism-based models, which is very beneficial in obtaining a highly accurate and feasible optimisation result. By looking at the advantages of using genetic algorithm in optimising the supercritical carbon dioxide process, we may suggest that the application of other complex-problem-solver algorithms and improved kinetic mechanism-based models would be very beneficial in the advanced study of this area.

Reference

Bashipour F., Ghoreishi S.M., 2012, Experimental optimization of supercritical extraction of β-carotene from Aloe barbadensis Miller via genetic algorithm, Journal of Supercritical Fluids 72, 312-319.

Chrastil J., 1982, Solubility of solids and liquids in supercritical gases, Journal of Physical Chemistry 86, 3016 -3021.

Dos Santos W., Silva E.A., Taranto O.P., 2013, Supercritical fluid extraction from mango (Mangifera indica l.) leaves: experiments and modeling, Chemical Engineering Transactions 32, 2005-2010.

Duba K.S., Fiori L., 2015, Supercritical fluid extraction of vegetable oils: different approach to modeling the mass transfer kinetics, Chemical Engineering Transactions 43, 1051-1056.

Fiori L., Basso D., Costa P., 2009, Supercritical extraction kinetics of seed oil: a new model bridging the ‘broken and intact cells’ and the ‘shrinking-core’ models, Journal of Supercritical Fluids 48 (2), 131-138.

Gordillo M.D., Blanco M.A., Molero A., Martinez de la Ossa E., 1999, Solubility of the antibiotic Penicillin G in supercritical carbon dioxide, Journal of Supercritical Fluids 15, 183-190.

Goto M., Roy B.C., Hirose T., 1996, Shrinking-core leaching model for supercritical-fluid extraction, Journal of Supercritical Fluids 9, 128-133.

Hasan N., Farouk B., 2013, Mass transfer enhancement in supercritical fluid extraction by acoustic waves, Journal of Supercritical Fluids 80, 60-70.

Hatami T., Glisic S. B., Orlovic A. M., 2012, Modelling and optimization of supercritical carbon dioxide of St. John’s Wort (Hypericum perforatum L.) using genetic algorithm, Journal of Supercritical Fluid 62, 102-108.

Hatami T., Meireles M.A.A., Zahedi G., 2010, Mathematical modeling and genetic algorithm optimization of clove oil extraction with supercritical carbon dioxide, Journal of Supercritical Fluids 51, 331-338.

Holland J.H., 1975, Adaptation in Natural and Artificial Systems, University of Michigan Press, Ann Arbor, United States.

Keshmiri K., Vatanara A., Yamini Y., 2014, Development and evaluation of a new semi-empirical model for correlation of drug solubility in supercritical CO2, Fluid Phase Equilibria 363, 18-26.

Liza M.S., Abdul Rahman R., Mandana B., Jinap S., Rahmat A., Zaidul I.S.M., Hamid A., 2010, Supercritical carbon dioxide extraction of bioactive flavonoid from Strobilanthes crispus (Pecah Kaca), Food and Bioproducts Processing 88, 319-326.

Machmudah S., Annt Sulaswatty, Mitsuru Sasaki, Motonobu Goto, Tsutomu Hirose., 2006, Supercritical CO2 Extraction of Nutmeg Oil: Experiments and Modeling, Journal of Supercritical Fluids 39, 30-39.

Mendez-Santiago J., Teja A.S., 2000, Solubility of Solids in Supercritical Fluids: Consistency of Data and a New Model for Cosolvent Systems, Ind. Eng. Chem. Res 39, 4767-4771.

Mezzomo N., Martínez J., Ferreira S.R.S., 2009, Supercritical fluid extraction of peach (Prunus persica) almond oil: Kinetics, mathematical modeling and scale-up, The Journal of Supercritical Fluids 51 (1), 10-16.

Pilavtepe M., Yesil-Celiktas O., 2013, Mathematical modeling and mass transfer considerations in supercritical fluid extraction of Posidonia oceanica residues, Journal of Supercritical Fluids 82, 244-250.

Piras A., Rosa A., Falconieri D., Porcedda S., Dessì M.A., Marongiu B., 2009, Extraction of oil from wheat germ by supercritical CO2. Molecules, 14 (7), 2573-2581.

Rahimi E., Prado J.M., Zahedi G., Meireles M.A.A., 2011, Chamomile extraction with supercritical carbon dioxide: Mathematical modeling and optimization, Journal of Supercritical Fluids 56, 80-88.

Salgin U., Salgin S., 2013, Effect of main process parameters on extraction of pine kernel lipid using supercritical green solvents: Solubility models and lipid profiles, Journal of Supercritical Fluids 73, 18-27.

Sharif K.M., Rahman M.M., Azmir J., Mohamed A., Jahurul M.H.A., Sahena F., Zaidul I.S.M., 2014, Experimental design of supercritical fluid extraction - A review, Journal of Food Engineering 124, 105-116.

Sovová H., 2005, Mathematical model for supercritical fluid extraction of natural products and extraction curve evaluation, Journal of Supercritical Fluids 33, 35-52.

Thana P., Machmudah S., Goto M., Sasaki M., Pavasant P., Shotipruk A., 2008, Response surface methodology to supercritical carbon dioxide extraction of astaxanthin from Haematococcus pluvialis, Bioresource Technology 99, 3110-3115.

Tomita K., Machmudah S., Quitain A.T., Sasaki M., Fukuzato R., Goto M., 2013, Extraction and solubility evaluation of functional seed oil in supercritical carbon dioxide, Journal of Supercritical Fluids 79, 109-113.

Zahedi G., Elkamel A., Lohi A., 2010, Genetic algorithm optimization of supercritical fluid extraction of nimbin from neem seeds, Journal of Food Engineering 97, 127-134.

Zhao S., Zhang D., 2013, Supercritical fluid extraction and characterisation of Moringa oleifera leaves oil, Separation and Purification Technology 118, 497-502.