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Kinetic Modeling and Parameters Identification Based on Metaheuristic Optimization Techniques for Extraction Process of *Marrubium vulgare* L. Essential Oil

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ABSTRACT

Recently, increasing attention has been directed to the isolation of natural active components from various medicinal plants. In the present research, the extraction of essential oil from horehound (*M. vulgare* L.) is presented. Effects of mass ratio and particle size on the process performance were studied and kinetics were determined. The chemical composition of the volatiles present in *M. vulgare* L. was evaluated for the sample extracted in the optimum conditions (mass ratio, 3 kg m^{-3} and particle size,0.1< d<0.63 mm) by using GC–MS. Eugenol (21.5%), *β*-Caryophyllene (11.5%) and β-bisabolene (10.3 %) were the major constituents found. Experimental data were fitted into three mathematical models having one and two time constants, in order to describe the extraction behaviour. The obtained coefficients of correlation show that the predicted and experimental data were in good agreement (0.9954< R<0.9982). In all cases the model constants have been found to change with mass ratio and particle size. The study was also an opportunity to improve the performance of two evolutionary algorithms, Genetic Algorithm (GA) and Particle Swarm Optimization (PSO), for identification of kinetic parameters with a satisfactory accuracy. The presented approach can be helpful for modeling and optimization of further extraction processes.

Keywords: Genetic algorithm, Grinding effect, Parameter identification, Particle swarm optimization Mass ratio effect.

INTRODUCTION

Kinetic modeling is one of the crucial issues, whose objective is making an accurate prediction of the extraction process performance and is a pivotal element for the process design, development, and advanced control.

Marrubium vulgare, commonly known as horehound, is a well-known herbal medicine of mint family, native to Europe, Western Asia, and North Africa and is cultivated worldwide as a source for food flavoring and for medicinal purposes (Letchamo and Mukhopadhyay, 1997; Sahpaz *et al*., 2002). Traditionally, it has been used to cure several diseases such as chronic coughs, bronchitis and whooping cough (Duke *et al.,* 2002). Thanks to the great importance of this medicinal plant, it has been the subject of several previous reports that have specially marked its antibacterial and antioxidant proprieties. Among the newest reviews: the papers of Morteza-Semnani *et al.* (2008), Masoodi *et al.* (2008), Kadri *et al.* (2011), Zawiślak (2012) and Abadi and Hassani (2013) deal with the composition of its oil and the antibacterial and antioxidant

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activities of *M. vulgare* L. from Iran, India, Tunisia, Poland and Algeria, respectively.

Process of extracting of Essential Oils (EO) containing bioactive compounds from their natural sources is a milestone for the use of these compounds as ingredients and potential additives in food, pharmaceutical and cosmetic industries (Goudarzi *et al*., 2011; Rasooli *et al*., 2002). Various techniques have been used for extraction of the essential oil: hydrodistillation, steam distillation, solvent extraction, and supercritical fluid extraction (Naef, 2011). It has been found that the properties of essential oils extracted by these methods considerably vary and highly depend on the method used (Okoh *et al.,* 2010). In addition, it is known that the concentrations of bioactive compounds in extracts are generally low, reason why efforts are made to increase the extraction yield while keeping process costs as low as possible by optimizing the significant operating variables, in order to maximize the extraction yield (Milić *et al.,* 2012).

Most of the existing papers interested in EO extraction are local in treating the yield, biological activities, and chemical composition. However, kinetic modeling has not been widely studied. In spite of its importance in the fundamental understanding, optimization, control, and conception of the industrial process (Milojević *et al.,* 2013). Authors such as Koul *et al.* (2004), Cassel *et al.* (2009) and Milojević *et al.* (2013) have reported the kinetic modeling of extraction process of E.O. isolated from a large range of plant species (Pornpunyapat *et al.,* 2011).

Moreover, the modeling of the extraction kinetics usually requires fitting the developed models with experimental data which leads to a parameter identification problem. Generally, this problem can be formulated as an optimization problem which seeks the least possible error between experimental data and model outputs. Unfortunately, some of the classical methods used in these cases e.g. Levenberg–Marquardt and simplex, may be unable to find the global minimum in presence of local minima and the identification of the model parameters can suffer for global convergence problems according to the limits of those algorithms (Rezazi *et al.,* 2016; Keyvanloo, 2012). Therefore, to overcome these limitations, metaheuristic algorithms have been implemented to solve different optimization problems (Elsayed *et al*., 2014).

Genetic Algorithm (GA), originally proposed by Holland (1975), is a stochastic method to solve the optimization problems defined by fitness criteria, applying the evolution hypothesis of Darwin and different genetic functions, i.e. crossover and mutation. (Nekoei *et al*., 2011; Nekoei *et al*., 2015). Over the last two decades, there have been many applications of GA in chemical engineering to solve different problems and optimization plans (Mohammadhosseini *et al*., 2012).

Particle Swarm Optimization (PSO) is a relatively recent heuristic search technique whose mechanics are inspired by the swarming or collaborative behavior of biological populations. This latter is similar to the GA in the sense that these two evolutionary heuristics are population-based search techniques. Many practical applications of PSO have been explored, including control of dynamical systems, data mining, transport problems, combinatorial optimization, and many others (Poli, 2007; Umarani and Selvi, 2010; Najjarzadeh, 2008; Hassan *et al*., 2004).

The main purpose of this study was to investigate the effect of two crucial factors, namely, mass ratio and particle size, on the extraction yield of hydrodistillation process performed on the aerial part of *M. vulgare L.*, in order to improve the operating efficiency and to maximize the performance of the extraction process by analyzing the variation of process yield with time. Furthermore, the present study aimed to deal with modeling studies as well as the identification of the models parameter values that provide the best fitness to measured data by using GA and PSO

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algorithms, proposed as new approaches for nonlinear parameter estimation in the case of modeling of EO extraction process.

MATERIALS AND METHODS

Plant Material

Mature whole *M. vulgare* L. plant was collected in northern Algeria (Rezarza, Medea) between March and May 2013. The plant material having moisture content of 48–50% was dried to constant weight in the drying oven, which was kept at a temperature of 30°C, for 6 days and then stored in a dry place prior to use. The maps of the sample location (Rezarza area) and the study area are shown in Figure1 by using ArcGIS 10.0 and Google Earth.

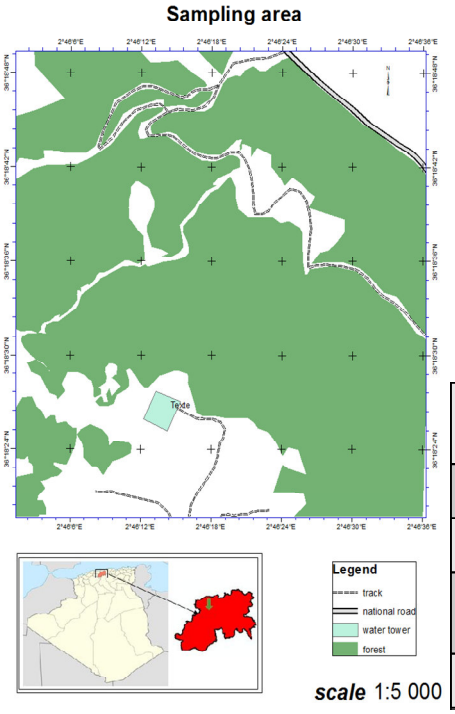
Essential Oils Isolation Procedure

Hydrodistillation processes were performed using a Clevenger-type apparatus, according to the method recommended by the European Pharmacopoeia (1983). The samples of *M. vulgare* L. leaves were swollen with distilled water for approximately 3 hours until the oil quantity in the extractor did not increase. In order to study the kinetic aspect of the extraction, the essential oils were collected every 20 minutes using the separator funnel. All the essential oils were dried using anhydrous sodium sulfate and, finally, stored in the dark glass bottle at 4°C. The percentage of extracting oil was calculated as follows:

The yield of essential oil (%)= [Essential oil weight (g)/Plant weight (g)]×100.

Effects of Process Factors on EO Yields

In order to improve the extraction kinetic and experimental process conditions, the Ratio of solid to liquid Effect (RE) on the EO yield was tested by using three mass ratios values (3, 5 and 7 kg m^{-3}). Weighed dried samples of crushed plant having a fixed particle size (1.25< d< 2 mm) were investigated. The mass ratio (P) is defined as the ratio between the mass of the sample



Name of the sampling area	Rezarza, Medea, Algeria
Latitude	36.307927°
Longitude	2.770438°
Height from the sea level	618 m
Altitude	891 m

Figure 1. Descriptive map of the sampling area (Rezarza, Medea).

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(m) and the Volume of solvent used (V) and is expressed by the following equation:

$$P(\%) = \frac{m}{V} \times 100 \quad (1)$$

Furthermore, the Effect of Grinding (GE) on the essential oils yield was also studied. Accordingly, extraction process was carried out on the dried plant by using four different particle sizes: (d> 2 mm, 1.25< d< 2 mm, 0.63< d< 1.25 mm, 0.1< d< 0.63 mm), while the optimum mass ratio found in the first set of experiments was investigated and the same conditions of sampling, storage, and extraction were applied to the whole samples.

Analysis Method

Gas Chromatography (GC) Analysis

The essence produced from horehound was diluted in n-hexane (1:100) and analyzed using a HP 5980 apparatus equipped with FID and DB5 fused silica capillary column (30 m×0.25 mm, film thickness 0.25 µm). Analytical conditions were: injector and detector temperature, 240 and 260 °C, respectively; oven temperature programmed from 60 to 250°C at 2 °C min^{-1}, then, held isothermal at 250°C for 10 minUTES; Helium as carrier gas was used at a flow rate of 0.8 mL min^{-1} .The diluted EO (1.0 µL) was injected in the splitless mode (1/60). Quantitative data were obtained from GC peaks area percent.

Gas Chromatography/Mass Spectrometry (GC/MS) Analysis

The composition of EO was determined by Gas Chromatography coupled to Mass Spectrometry (CG/MS) technique. A Hewlett-Packard 5890 gas chromatograph was employed. It was coupled to a 5973A mass spectrometer; A DB5-MS fused silica capillary column (30 m×0.25 mm id, film thickness 0.25 µm) was employed. GC conditions used were: isothermal 60°C, 8 minutes, programmed heating from 60°C to 250°C at 2 °C min^{-1} isothermal, 30 min. The injector was maintained at 250°C. Helium was the carrier gas at 0.5 mL min^{-1}; the sample (1.0 µL) was injected in the split mode (1/20). MS conditions were as follows: ionization voltage, 70 eV; scan range, 35-500 uma. The identification of the compounds was performed by comparing their retention indices and mass spectra with those found in the literature (Adams, 2001) and supplemented by the Wiley and QuadLib 1607 GC–MS libraries.

Mathematical and Numerical Methods

Three models were tested in order to describe the experimental data on the extraction of essential oils from *M. vulgare* L.: two phenomenological models presented by Milojević *et al.* (2013) and Milić *et al.* (2012) describing the kinetics of extraction of essential oils, the first one is a model of simultaneous washing and diffusion (2) whereas the second one is a simplified model called: Model of instantaneous washing followed by diffusion (3). The previous authors assumed that the models were based on two main processes: "washing" of the essential oil from external surfaces of the particles, and "diffusion" of the essential oil from the inside of the plant particles to their external surfaces (Rezazi *et al.,* 2016).Those models have been verified by: Milojević *et al.* (2008) on the juniper berries, Stanisavljević *et al.* (2010) using the laurel leaves, Kapás *et al.* (2011) for fennel seeds, and Pornpunyapat *et al.* (2011) using the agarwood.

On the other hand, a pseudo-first order kinetics model (4) was also presented by several authors using different plant materials: leaves of thyme (*Thymbra spicata* L.) (Hanci *et al.,* 2003), lemon grass (*Cymbopogon* spp.) (Koul *et al.,* 2004), celery (*Apium graveolens* Linn.) (Sowbhagya *et al*., 2007), and flowers of lavender (*Lavandula angustifolia* Mnch) (Milojević *et al.,* 2013).

Kinetic Models Description

All the mathematical models used in the present study are based on some general assumptions: (i) Plant particles are considered to have properties including shape, size and the initial essential oil

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content (Milojević *et al.,* 2013); (ii) The concentration gradients in the fluid phase develop at scales higher than the particle size; (iii) The solvent flow-rate is uniformly distributed in every section of the extractor (Grosso *et al.,* 2010); (iv) Some of the essential oil is located on the external surfaces of the vegetable particles, f, and the rest is uniformly distributed throughout the plant particles, (1-*f*); (v) The essential oil is considered as a single component; (vi) The effective coefficient of diffusion through plant particles is constant, and (vii) There is no resistance to the mass transfer of essential oil from the external surfaces of the plant particles (Milojević *et al.,* 2013).

Model 1: Model of Simultaneous Washing and Diffusion

The mathematical model describes a first-order kinetic; the two processes of washing and diffusion have been presented by the following formula (Sovova *et al.,* 2006):

$$\frac{C}{C_\infty} = 1 - f.e^{-k_1 t} - (1-f).e^{-k_2 t} \quad (2)$$

Where, C is the concentration of essential oil existing in the plant particles (g 100 g^{-1}) at time t, C_∞ is the essential oil concentration at the end of the extraction, t is the time of the extraction process, f is the fraction of the essential oil washed from the broken plant cells on the particle surfaces, k_1 and k_2 are the rate constants for both of washing and diffusion, respectively. The portion of the essential oil that will be washed is supposed to be unchanged.

Model 2: Model of Instantaneous Washing Followed by Diffusion

A simplified model has been previously derived for the recovery of essential oil from plant materials if the washing phase is assumed faster than the diffusion and occurs instantaneously ($k_1 \to \infty$) (Milojević *et al.,* 2008). Therefore, Equation (2) becomes:

$$\frac{C}{C_\infty} = 1 - (1-f).e^{-k_2 t} \quad (3)$$

Model 3: Model of Pseudo-First Order Kinetics

If f = 0, which means that washing does not occur, then, the essential oil concentration increases exponentially due to diffusion, so, Equation (3) can be rewritten as follows:

$$\frac{C}{C_\infty} = 1 - e^{-k_2 t} \quad (4)$$

Goodness of Fit

The performances of the tested models were statistically measured by the Root Mean Squared Error ($RMSE$), Mean Squared Error (MSE), Average Absolute Deviation [$AAD(\%)$] and the coefficient of correlation (R) (Rezazi *et al.,* 2016), which were computed using the following equations:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_{\exp} - y_{cal})_i^2} \quad (5)$$

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_{\exp} - y_{cal})_i^2 \quad (6)$$

$$AAD(\%) = \frac{1}{N}\sum_{i=1}^{N}\left|y_{\exp} - y_{cal}\right|_i \quad (7)$$

$$R = \frac{\sum_{i=1}^{N}(y_{\exp} - \bar{y}_{\exp})(y_{cal} - \bar{y}_{cal})}{\sum_{i=1}^{N}(y_{\exp} - \bar{y}_{\exp})^2 \sum_{i=2}^{N}(y_{cal} - \bar{y}_{cal})^2} \quad (8)$$

Where $y_{cal} = \alpha\, y_{\exp} + \beta$ (9)

$y_{\exp} = (C/C_\infty)_{\exp}$ and $y_{cal} = (C/C_\infty)_{cal}$ (10)

RESULTS AND DISCUSSION

Effect of Mass Ratio on EO Yield

Kinetic study of the variation of yield with time for different mass ratios is examined

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and presented in Figure 2-a. Investigations treated a set of mass ratios (3, 5 and 7 kg m^{-3}) and all the samples had similar particle sizes (1.25< d< 2 mm). Results showed that the maximum extraction yield of essential oil was obtained when using the ratio of 3 kg m^{-3}. Further increase of solid amount had no significant impact on the extracting yields. The solid to solvent ratio effect is a crucial factor for obtaining the maximum extractability by reducing up or down the ratio between the mass of the sample and the volume of the solvent (Shogren *et al.,* 2006).

Effect of Grinding Degree on EO Yield

To study the effect of grinding on the extraction yields, the mass ratio of 3 kg m^{-3} fixed as the optimum ratio. The variation of EO yield against time was plotted for different particle sizes in Figure 2-b. It was observed that the extraction yield increases with decreases in particle size and the optimum size that yielded higher oil extraction was 0.1< d< 0.63 mm. The main purpose of grinding is to reduce particle size and increase the surface area contributing to the EO diffusion during the extraction process (Hazwan *et al.,* 2012). The smaller particle size exhibits greater surface area that entails an increase in mass transfer between solid particles and solvent (Turker and Erdogdu, 2006; Franco *et al.,* 2007).The smaller sized particles probably associated with more intense cell wall breakage and led to higher extraction yields (Salgina *et al.,* 2006; Ozkal *et al.,* 2005). However, the lower bound of particle size has not been reported until now in any literature.

Essential Oil Composition

The results of the GC analysis- mass spectrometry of the chemical composition of *M. vulgare* L. EO extracted in the experimental conditions giving the high yield (mass ratio, 3 kg m^{-3} and particle size, 0.1< d< 0.63 mm) are presented in Table 1, wherein the identified compounds are listed in the order of predominance. A total of 28 compounds was identified which corresponds to a percentage of 97.72% relative to the set of constituent isolated. Eugenol appears as the major constituent of the EO (21.5%), followed by *β*-caryophyllene (11.5%), *β*-bisabolene (10.3%), *δ*-Cadinene (9.7%), *β*-Citronellol (9.13%), and Germacrene D (6.7%).

The obtained results seem to be in agreement with those reported by some other authors (Belhattab *et al.,* 2006; Nagy and Svajdlenka, 1998) for the essential oil omposition of *M. vulgare* L. from Algeria and Slovakia, rich in eugenol, *β*-bisabolene

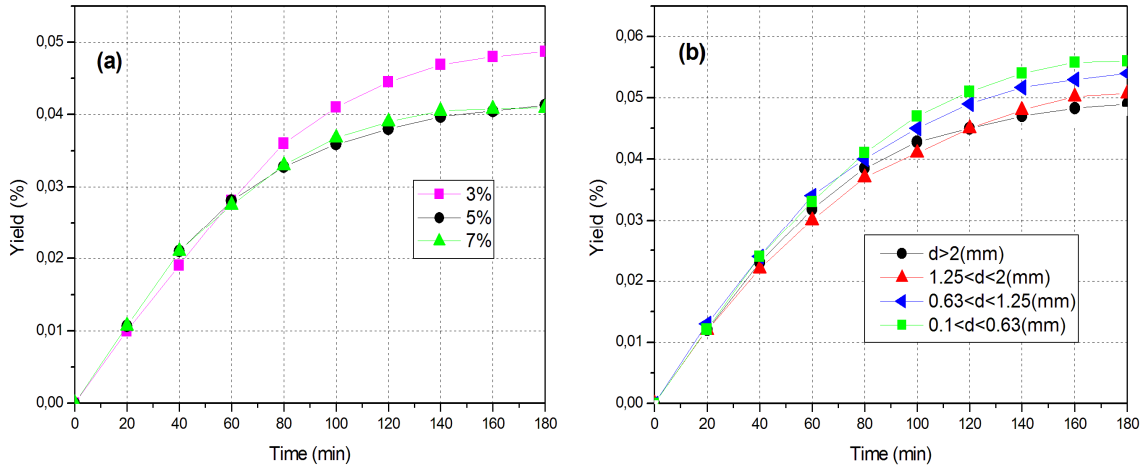

Figure 2. Operating conditions effects on the essential oils yield: (a) Effect of solvent to solid ratio, (b) Grinding effect.

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Table 1. Chemical composition of *M. vulgare* L. essential oil (% area of GC–MS analysis).

N°	Compound	*RI*[a]	(%) Area	Method of identification
1	Trans-2-hexanal	854	0.65	RI, GC–MS
2	Heptanal	899	0.1	RI, GC–MS
3	*α*-Pinene	939	1.56	RI, GC–MS
4	Camphene	953	0.49	RI, GC–MS
5	Sabinene	976	0.3	RI, GC–MS
6	Myrcene	991	2.1	RI, GC–MS
7	Octanol-3	997	2.3	RI, GC–MS
8	*p*-Cymene	1026	2.74	RI, GC–MS
9	1,8-Cineole	1033	3.25	RI, GC–MS
10	Nonanal	1098	1.3	RI, GC–MS
11	Linalool	1098	2.1	RI, GC–MS
12	*α*-Thujone	1102	2.39	RI, GC–MS
13	Camphor	1143	0.97	RI, GC–MS
14	*β*-Citronellol	1228	9.13	RI, GC–MS
15	Geraniol	1255	0.98	RI, GC–MS
16	carvacrol	1298	1.8	RI, GC–MS
17	Eugenol	1356	21.5	RI, GC–MS
18	*α*-Copaene	1376	1.12	RI, GC–MS
19	*β*-Bourbonene	1384	1.76	RI, GC–MS
20	*β*-Elemene	1391	0.15	RI, GC–MS
21	*β*-Caryophyllene	1418	11.5	RI, GC–MS
22	*α*-Hummulene	1440	1.3	RI, GC–MS
23	Germacrene D	1480	6.7	RI, GC–MS
24	*β*-bisabolene	1509	10.3	RI, GC–MS
25	*α*-Muurolene	1307	0.3	RI, GC–MS
26	*γ*-Cadinene	1512	0.45	RI, GC–MS
27	*δ*-Cadinene	1524	9.7	RI, GC–MS
28	Trans-nerolidol	1564	0.78	RI, GC–MS
Total identified			97 .72	
Yield (g 100 g^{-1} dry weight)			0.0487	
Monoterpene hydrocarbons			7.19	
Oxygenated monoterpenes			19.65	
Sesquiterpene hydrocarbons			43.28	
Oxygenated sesquiterpenes			0.78	
Others compounds			26.82	

[a] *RI*= Retention Indices on DB-5MS.

and *β*-caryophyllene. However, comparing the chemical compositions of the EO studied in this work with the one from Tunisia, we found that Tunisian oil was characterized by γ-eudesmol (11.93%), γ-citronellol (9.90%), citronellyl formate (9.50%) and germacrene D (9.37%) (Kadri *et al.,* 2011). Khanavi *et al.* (2005) reported that the EO of Iran was characterized by *β*-bisabolene, *β*-caryophyllene, germacrene D and *E*-*β*-farnesene. Whereas, *β*-bisabolene, *δ*-cadinene and iso-caryophyllene were the main compounds of *M. vulgare* from other region of Iran (Morteza-Semnani *et al.,* 2008). (E)-2-hexenal, *α*-humulene and germacrene D were reported as the main components of *M. vulgare* growing in Lithuania (Weel *et al.,* 1999).

Mathematical Modeling

Genetic Algorithm Development Procedure

The Genetic Algorithm (GA) is a stochastic search technique based on the mechanism of natural selection and natural

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genetics, which is applied to solve different types of optimization problems that are not well suited for standard optimization algorithms (Vatani *et al.,* 2014). The general flowchart of GAs is shown in Figure 3.

In GAs, the solution procedure starts with an initial set of random candidate solutions called population and each individual in the population is called a chromosome. A chromosome is a set of various segments (called genes) that represent the value of decision variable. The chromosomes evolve through successive iterations, called generation. During each generation, new chromosomes called offspring are formed by crossover and mutation, then, they are compared against each other according to a measure called fitness. Algorithm computes fitness function of each chromosome and selects those that have lower objective function as parents (Boozarjomehry and Mansoori, 2007).

Particle Swarm Optimization (PSO)

Particle Swarm Optimization (PSO) is a robust stochastic optimization technique based on the movement and intelligence of swarms. PSO is first introduced by Kennedy and Eberhart in 1995 (Russell and James, 1995). It was inspired by social behavior of animals living in swarms, including bird flocking or fish schooling (Wei-Der and Shun-Peng, 2010).

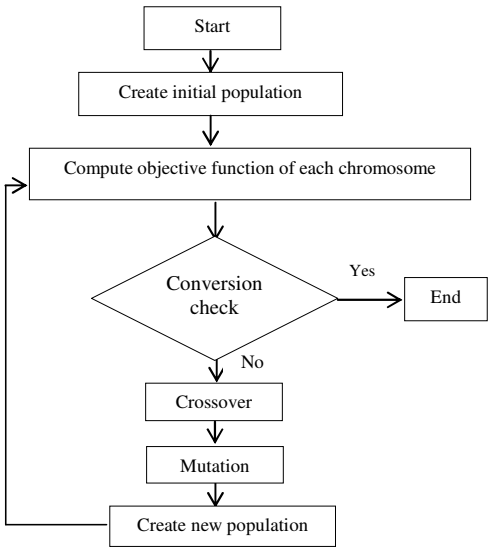

Figure 3. Flowchart of genetic algorithm.

Particle swarm optimization uses particles which represent potential solutions of the problem. Each particle is treated as a point in a search space which adjusts its "flying" according to its own flying experience as well as the flying experience of other particles. Equation (11) is used to calculate the position and velocity of each particle updated at discrete intervals:

$$\begin{cases} v_{id}^{\,t+1} = w v_{id}^{\,t} + c_1 r_1 \left(p_{id} - x_{id}\right) + c_2 r_2 \left(p_{gd} - x_{id}\right) \\ x_{id}^{\,t+1} = x_{id}^{\,t} + v_{id}^{\,t+1} \end{cases} \tag{11}$$

$$w = \frac{2}{\left|2 - c - \sqrt{c^2 - 4.c}\right|}, \; c = c_1 + c_2 \tag{12}$$

Where, t denotes the generation of algorithm running; w is the inertia weight which is called the constriction factor (Maurice, 1999) and is defined by Equation (12); d is dimension of the problem space; c_1 and c_2 are the acceleration constants depending on the relationship $c_1 + c_2 \le 4$; r_1 and r_2 are the uniformly generated random numbers in the range of [0, 1]; p_{id} is the best solution for this particle; p_{gd} is the best solution for all particles; $x_{id}^{\,t}$ is the i*th* particle in the t generation. In general, the value of each component in v can be restricted to the range $\left[-v_{\max}, v_{\max}\right]$ to control excessive roaming of particles outside the search space (Jiang *et al.,* 2007). The representation of the fitted Equations (2), (3), and (4) is shown in Figures 5 and 6, which illustrate the experimental and calculated extractions kinetic curves for the two studied effects by using GA and PSO, respectively. These figures clearly show that the curves correspond to the calculated points differ

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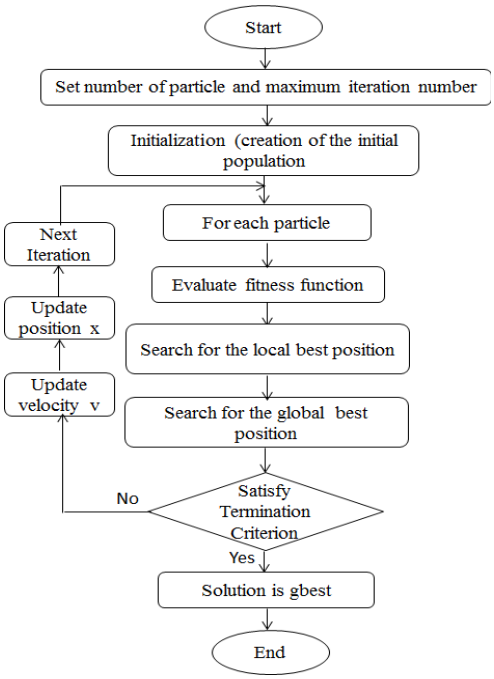

Figure 4. Flowchart of PSO algorithm.

slightly compared to those corresponding to the experimental measurements. This finding indicates that these models give a good representation of the extraction process behavior.

Parameter Identification of Models

In this section, the values of the kinetic parameters of the three models, given by Equations (2), (3) and (4) were estimated by using the function "*ga*" and "*pso*" of MATLAB. The estimation of optimal parameters was performed by connecting the modeling program and GA/PSO whose objective was to minimize the distance between the outputs of the model y_{cal} and the process outputs $y_{\exp}$. This leads to a minimization problem of the selected fitness function, which is the mean squared error between the experimental data and the derived results from the model (MSE) provided by Equation (6). The selected GA and PSO parameters obtained by trial and error are summarized in Table 2.

Figures 7-8 show the regression curves between the experimental values and the values predicted by the tested models. The plots were determined by using the function "*postreg*" of MATLAB representing comparisons between experimental results obtained in the first part of the study and the predicted results for the two tested effects: RE and GE on the EO yield.

Among the significant methods that can appreciate the predictive capability of each tested model, two are exploited in our study, i.e. the analysis of the regression curve between the experimental and predicted values as well as the assessment of the agreement vector values. It was proven that the proposed approaches give satisfactory results with satisfactory agreement vector values which are illustrated in Table 3.

The results given by the study of the grinding effect were shown to be the best ones, especially the second model which better fitted the experimental data than the other models and gave the best performances; [α, β, R] = [0,9785, 0,0082, 0,9982] in the case of modeling by using PSO. This shows the regression parameters values approaching the ideal [i.e. α=1 (slope), β=0 (y intercept), R=1 (correlation coefficient)] for the whole tested models.

The optimal kinetic parameters (k_1, k_2 and f) obtained using GA of the three tested models are summarized in Table 4.

Table 2. The control parameters used for running GA and PSO.

GA	PSO
Population size: 25	Population size: 25
Number of iteration: 150	Number of iteration: 150
Selection: Uniform stochastic	Social parameter c_1= 0.8
Crossover: Random	Cognitive parameter c_2= 1.2
Mutation: Gaussian	Speed factor w= 0.9

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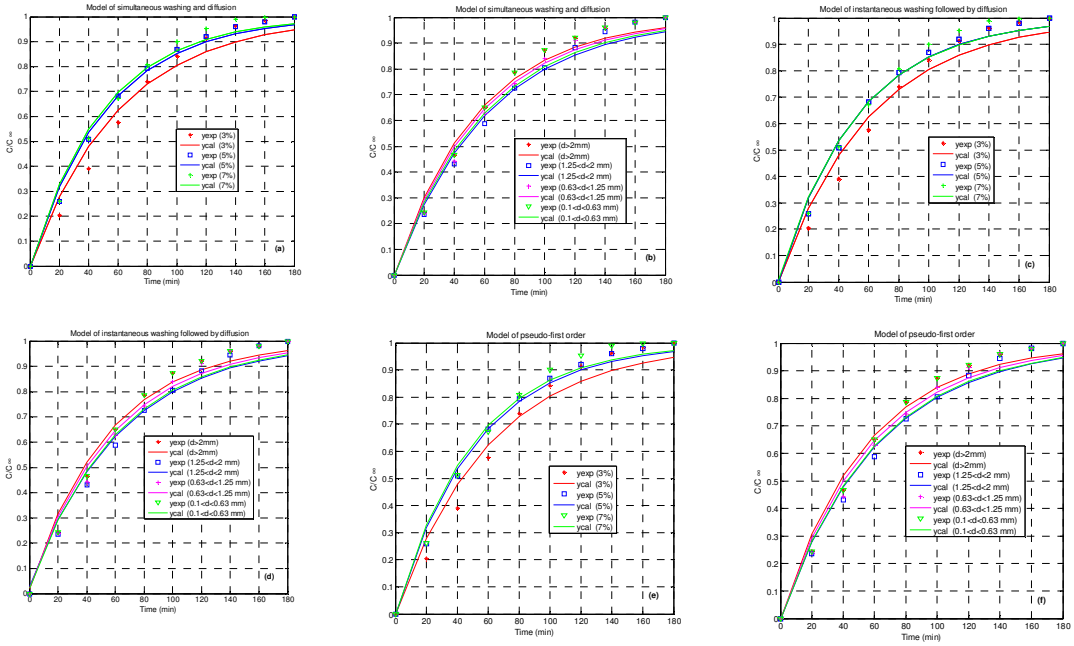

Figure 5. Plot of the experimental values and predicted values for the extraction yield vs. time: (a) Model 1 (RE), (b) Model 1 (GE), (c) Model 2 (RE), (d) Model 2 (GE), (e) Model 3 (RE), (f) Model 3 (GE).

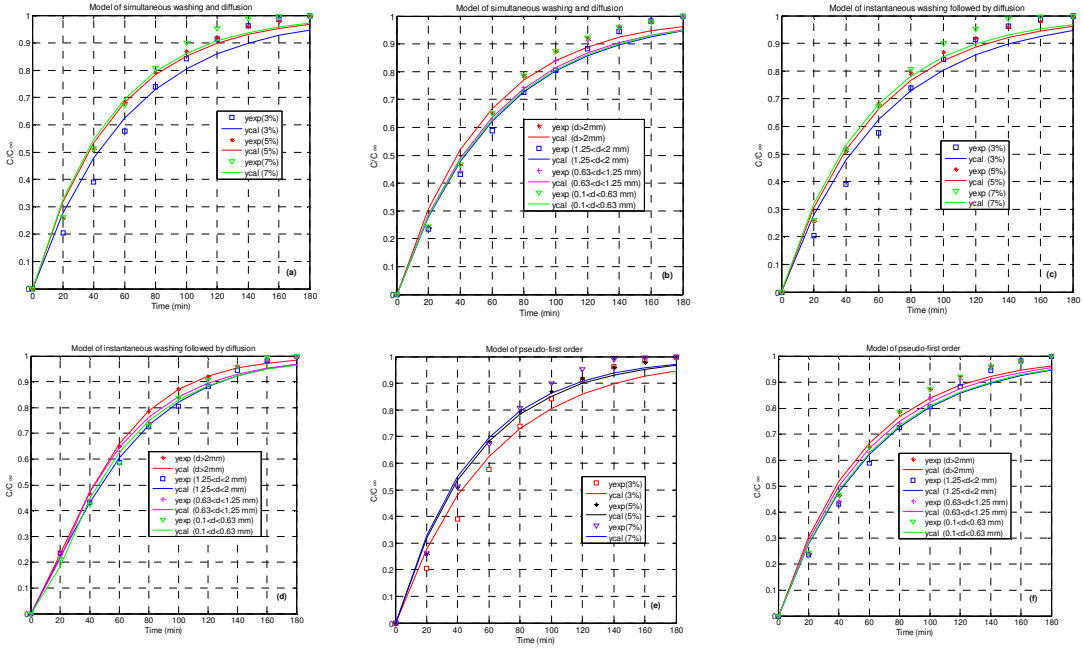

Figure 6. Plot of experimental values and predicted values for the extraction yield *vs*. time: (a) Model 1 (RE), (b) Model 1 (GE), (c) Model 2 (RE), (d) Model 2 (GE), (e) Model 3 (RE), (f) Model 3 (GE).

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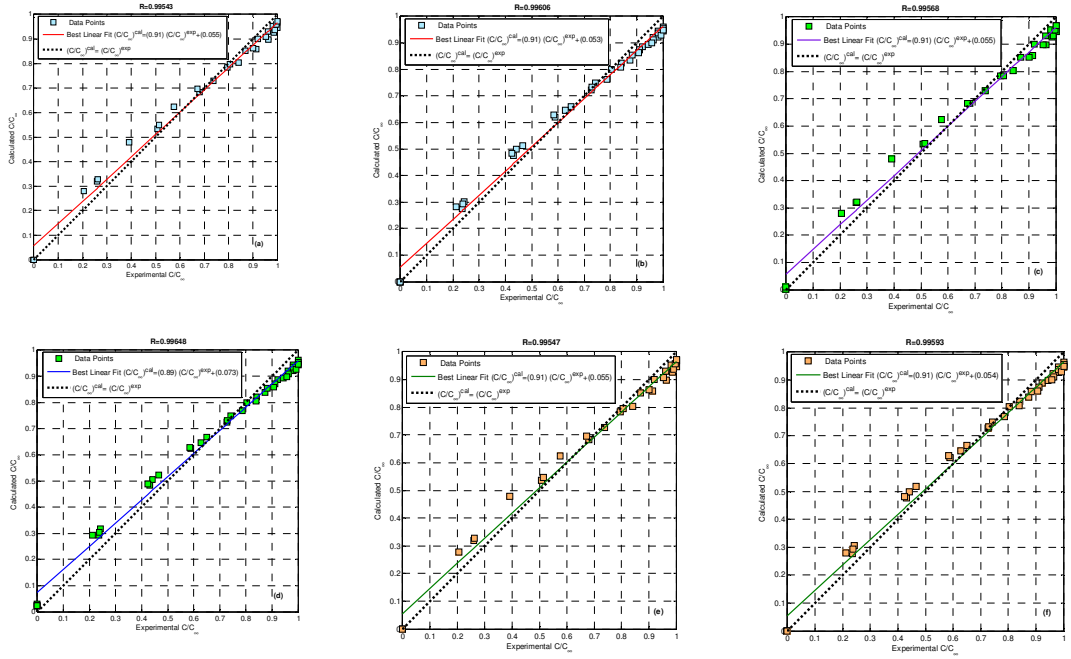

Figure 7 Regression curves of the kinetic models using GA: (a) Model 1 (RE), (b) Model 1 (GE), (c) Model 2 (RE), (d) Model 2 (GE), (e) Model 3 (RE), (f) Model 3 (GE).

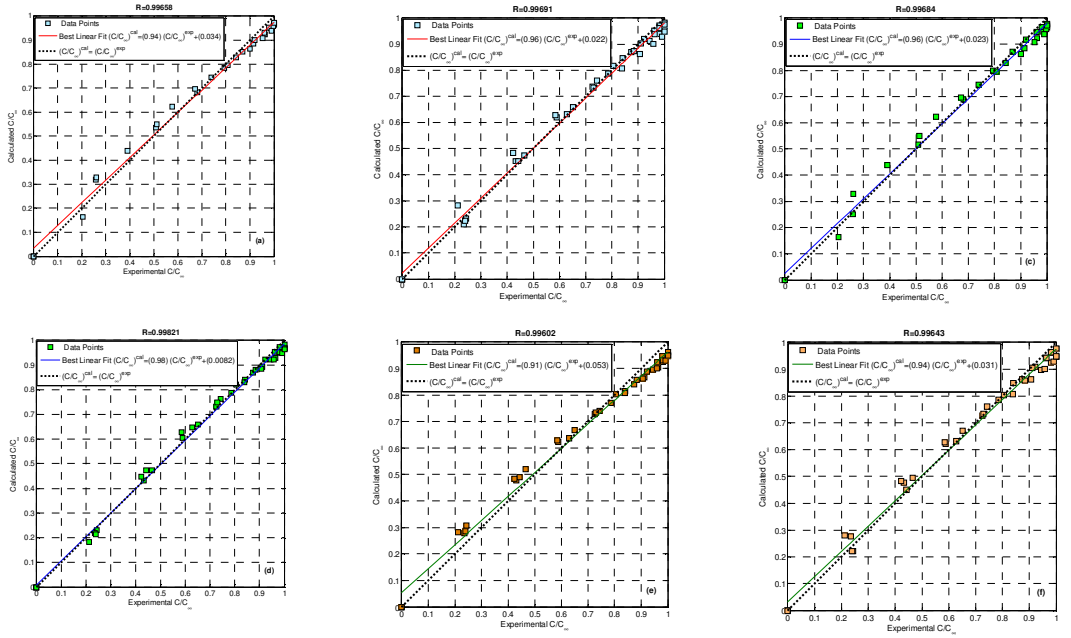

Figure 8 Regression curves of the kinetic models using PSO: (a) Model 1 (RE), (b) Model 1 (GE), (c) Model 2 (RE), (d) Model 2 (GE), (e) Model 3 (RE), (f) Model 3 (GE).

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Table 3. Validation agreement vector [α (slope), β (y intercept), R (correlation coefficient)] of the GA regression for the three tested models.

Effect		GA			PSO		
		Model 1	Model 2	Model 3	Model 1	Model 2	Model 3
Effect of Ratio of solid to Liquid (RE)	α	0.9107	0.9067	0.9106	0.9401	0.9558	0.9096
	β	0.055	0.0552	0.0546	0.0338	0.0234	0.0528
	R	0.9954	0.9957	0.9955	0.9966	0.9968	0.9960
Grinding Effect (GE)	α	0.9095	0.8861	0.9103	0.9593	0.9785	0.9445
	β	0.0527	0,0729	0.0537	0.0216	0.0082	0.0314
	R	0.9961	0,9965	0.9959	0.9969	0.9982	0.9964

Table 4. The optimal kinetic parameters of the fitted equations obtained using GA and PSO of the three tested models.

	Effect		Model 1			Model 2		Model 3
			K_1	K_2	f	K_2	f	K_2
GA	*RE*	3 kg m^{-3}	0.01614	0.01638	0.2377	0.01633	7.52007E-5	0.01626
		5 kg m^{-3}	0.01914	0.17266	1	0.01914	1.39434E-5	0.01915
		7 kg m^{-3}	0.01999	0.0196	0.81544	0.01899	0.00883	0.01986
	GE	d> 2(mm)	0.0191	0.01772	0.18664	0.01799	0.02006	0.0183
		1.25< d< 2 (mm)	0.02022	0.01593	0.0343	0.01578	0.03028	0.01625
		0.63< d< 1.25 (mm)	0.01731	0.01727	0.67675	0.01693	0.02459	0.01732
		0.1< d< 0.63 (mm)	0.01697	0.0162	0.4553	0.01613	0.02249	0.01646
PSO	*RE*	3 kg m^{-3}	0.01636	0.0159	0.9100	0.01627	0,0037	0,01632
		5 kg m^{-3}	0.01967	0.0176	0.74234	0.01815	0,0023	0,01914
		7 kg m^{-3}	0.02064	0.0193	0.39584	0.01899	0,00434	0,0199
	GE	d> 2(mm)	0.01936	0.01829	0,02501	0.01797	0.02160	0.0182479
		1.25< d< 2 (mm)	0.03120	0.01608	0,0170	0.01578	0.03021	0.01623331
		0.63< d< 1.25 (mm)	0.01761	0.01720	0,1896	0.01690	0.02450	0.0172820
		0.1< d< 0.63 (mm)	0.01661	0.01596	0.8300	0.01621	0.02080	0.0165110

Table 5. Statistical analyses of the error of the calculated results for the tested models.

		Effect	GA			PSO		
			Model 1	Model 2	Model 3	Model 1	Model 2	Model 3
AAD(%)	*RE*	3 kg m^{-3}	0.04868	0.0489	0.04868	0.02932	0.02930	0.03273
		5 kg m^{-3}	0.02236	0.02234	0.02236	0.02235	0.00875	0.03063
		7 kg m^{-3}	0.03361	0.03367	0.03654	0.03365	0.03363	0.03359
	GE	d> 2(mm)	0.03359	0.03279	0.03714	0.00699	0.00626	0.01584
		1.25< d< 2 (mm)	0.03125	0.03064	0.03754	0.02271	0.01416	0.03063
		0.63< d< 1.25 (mm)	0.03318	0.03321	0.03847	0.01292	0.02104	0.01238
		0.1< d< 0.63 (mm)	0.04241	0.04231	0.04729	0.04235	0.02604	0.04235
RMSE		*RE*	0.04187	0.04188	0.0427	0.03339	0.03003	0.04075
		GE	0.0407	0.04051	0.04486	0.02876	0.02141	0.03254

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The obtained values of the rate constants k_1 and k_2 indicate that the study of the *GE* on the extraction process offers more important values than those obtained for the *RE*. This means that both diffusion and washing were faster and the variation in the particle size affected more clearly the speed of the process characterized by greater values of the rate constants compared to those obtained in the study of the *RE*.

Models Performances

In order to identify clearly the qualities and the performances of the studied models, it is necessary to perform a statistical analysis of the various errors calculated by each model. Table 5 summarizes the errors of the predicted results for the three tested models, i.e. the [$AAD(\%)$] values along with the values of (*RMSE*) for *GE* and *RE* effects.

A global view of Table 5 indicates that all the obtained errors have an acceptable value (less than 0.1). It shows that the *RMSE* values obtained with the application of the simultaneous washing and diffusion model are the lowest and gave satisfactory deviations ranging from 0.02141to 0.04486 for the study of *GE* and *RE* effects, respectively.

According to the previous findings, the obtained simulation results confirm the accuracy of the parameters derived from the two algorithms having a high capacity of global search, with some differences in the convergence speed and computational efficiency. PSO is more robust in its operation and gives the higher performances with the use of few parameters.

CONCLUSIONS

This study indicated that the variables chosen, namely, particle size and ratio of solid to solvent, have a significant influence on the yield of essential oils. The results conclude that the plant crushing to an average size of $0.1< d< 0.63$ mm and using the mass ratio of 3 kg m^{-3} yield higher extraction rates. Particle size was found to be the most significant factor influencing the process. The results showed that the extraction process was governed by two parallel mechanisms having different characteristic times: A rapid diffusion (washing stage) from the broken cell walls close to the external surface of the particles, and a slower diffusion (diffusion stage) from the cells with intact walls located at the center of the particle. Moreover, the modeling of the extraction process of EO was investigated using three different mathematical models. The used models described well the extraction process and the identification procedure of the different kinetic parameter values based on the use of GA and PSO provided the best fit to the measured data and gave good performances ($0.9964< R <0.9982$). Due to the flexibility and the generality of particle swarm optimization, their introduction as an optimization technique ameliorates the quality of modeling compared to the classical mathematical method and it seems to be a useful technique with lots of potential in the determination of the optimum kinetic model corresponding to different extraction processes.

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مدل سازی سینتیک و شناسایی پارامتر مدل ها بر پایه روش های بهینه سازی ابتکاری برای فرایند عصاره گیری اسانس *Marrubium Vulgare* L.

س. رزازی، س. هانینی، س. سی-موسی، و س. عبدالملک

چکیده

اخیرا، به جدا سازی مواد و اجزای فعال گیاهان دارویی مختلف توجه روز افزونی می شود. در پژوهش حاضر، عصاره گیری اسانس از گیاه *M. Vulgare* L. مطالعه و ارایه شده است. اثر نسبت جرم (mass ratio) و اندازه ذرات روی عملکرد فرایند عصاره گیری بررسی شد و سینتیک آن تعیین شد. ترکیبات شیمیایی مواد فرّار موجود در *M. Vulgare* L. در نمونه های استخراج شده در شرایط بهینه (نسبت جرم برابر $3\ kg/m^3$ و اندازه ذرات $0.1<d<0.63\ mm$) با استفاده از گاز کروماتوگرافی/ اسپکترومتری جرمی(GC–MS) ارزیابی شد. ترکیبات اصلی عبارت بودند از یوژنول(۲۱/۵%)، β-Caryophyllene (۱۱/۵٪) و β-bisabolene (۱۰/۳٪). به منظور تشریح رفتار استخراج (عصاره گیری)، داده های آزمایش به سه مدل که یک و دو ضریب ثابت زمانی(time constants) داشتند برازش شدند. ضرایب همبستگی به دست آمده نشان می دهد که داده های پیش بینی شده و اندازه گیری شده مطابقت خوبی با هم دارند($0.9954<R<0.9982$). در همه موارد، معلوم شد که ضرایب مدل با نسبت جرم و اندازه ذرات تغییر می کند. در این پژوهش، عملکرد دو الگوریتم تکاملی برای شناسایی پارامتر های سینتیک یعنی الگوریتم ژنتیکی (GA) و بهینه سازی ازدحام ذرات (particle swarm optimization)، با دقتی مناسب بهبود داده شد. به این قرار، روش ارایه شده در این تحقیق می تواند برای مدل سازی و بهینه سازی دیگر فرایندهای استخراج (عصاره گیری) مفید باشد.

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