

Extraction Performance of Essential Oils by Hydrodistillation Using Mathematical Models: A Systematic Review

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Abstract: Essential oils are complex mixtures of volatile organic compounds valued for their antimicrobial and antioxidant properties, with widespread applications in the food, pharmaceutical, and cosmetic industries. Among the various extraction techniques employed, hydrodistillation remains one of the most widely used methods. The extraction yield of essential oils by hydrodistillation is influenced by multiple factors, and quantifying these through mathematical modelling is critical for assessing the efficiency, efficacy, and economic viability of the process. This systematic review aimed to identify, evaluate, and synthesize scientific studies that applied mathematical models to calculate the hydrodistillation extraction yield of essential oils. A systematic search was conducted across four databases - Scopus, ScienceDirect, SciELO, and EBSCO - covering literature published up to April 2023. Studies were screened and selected based on pre-defined eligibility criteria in accordance with PRISMA guidelines. Seventeen studies met the inclusion criteria, reporting the hydrodistillation of essential oils from nineteen plant species using various plant parts including leaves, flowers, fruits, and roots. Of these, ten studies applied response surface methodology, four used kinetic modelling, and three employed data mining algorithms. Variables influencing extraction yield were classified into agro-climatic, conditioning, and exploitation factors. Response surface models with varied design types and kinetic models were the most frequently applied approaches; however, an emerging trend toward data mining algorithms was observed. These findings provide a structured overview of current modelling approaches for essential oil extraction and highlight the growing potential of machine learning-based methods as promising tools for optimizing hydrodistillation processes.

Keywords: Hydrodistillation, Essential oils, Extraction yield, Response surface methodology, Kinetic modelling, Data mining, Mathematical models, Systematic review

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Introduction

Essential Oils (EO) are highly concentrated aromatic compounds formed in the secondary metabolism of plants, are stored in the glandular trichome cells; obtained from flowers, leaves, stems and roots [1-4]. They are oily and volatile liquid fractions consisting of a mixture of more than 100 chemical compounds, include terpenoids (monoterpenes and sesquiterpenes) and

low molecular weight compounds (alcohols, aldehydes, ketones, lactones, acetals, oxides, esters and phenols) [5, 6]. Due to their intense and unique flavors, they are used to enhance the taste and aroma of food products; features that contribute to food preservation and extend its shelf life [7-11]. In addition, due to its antioxidant and anti-inflammatory properties, have health benefits, as therapeutic effects, promote digestion, improve circulation, and reduce stress [12-18]. Therefore, they are an alternative to synthetic additives, such as artificial flavors and preservatives, which are used in the food industry and is an option for consumers looking for clean label products [19-21].

The techniques for obtaining EO include: distillation with organic solvents, microwave-assisted distillation, gravity and microwave hydrodiffusion, enfleurage, expression, supercritical carbon dioxide extraction, hydrodistillation, steam distillation, and ultrasound extraction [22]. Steam distillation is based on allowing steam to pass through the plant material, causing the EO to evaporate. Subsequently, both the steam and the EO are condensed and separated [23-25]. The expression consists of squeezing the plant material to release the EO, which is then collected [26-28]. With solvents it uses ethanol (It uses ethanol as solvents), hexane [29] Supercritical CO₂ [30-31], then the solvent evaporates and leaves the oil. Enfleurage, consists of placing the plant material in a fat or oil, the plant material is removed and the fat or oil is dissolved in alcohol to extract the EO [32-33] Hydrodistillation is a method using water and steam [34], however, there are variants of the heat transfer method such as microwave and infrared hydrodiffusion [35]. This is a type of steam distillation in which the plant material is placed in a still and water is added [36]; the still is heated, causing the water to boil and the steam to pass through the plant material, carrying with it the EO, the mixture of steam and EO passes through a condenser, where it cools and condenses back to liquid [37]. However, some methods are more efficient than others, differentiating conventional methods such as steam distillation, hydrodistillation, hydrodiffusion and solvent extraction from non-conventional methods such as solventless microwave extraction, subcritical liquid extraction and supercritical fluid extraction, which produce higher quality oils [38-41].

The extraction yield, maximum volume of EO extracted by weight of the sample, relates the maximum amount of oil that can be obtained from the plant material, depending on the extraction technique [42] and established parameters [43, 34], as drying [44], soil and climate, milling process [45], time of growth and type of plant parts [46], even metabolic engineering can enhance performance [47].

Mathematical models are expressions of the processes that govern events that cannot be identified, controlled, or understood [48], and involve the quantification of data [49]. It is a necessary and effective tool for decision making [48]. Therefore, it is used to describe the effect of the variables involved in the processes of obtaining essential oils [50]. Response Surface Methodology (RSM) is a combination of regression analysis and experimental design [51] which was proposed by Box and Wilson in 1951, allows locating optimal values for the variables [52] and its useful instruments for the studio, development and optimization of a varied extent of systems [53] such as slope reliability analysis [54], mixing ratios [55], biological wastewater treatment processes [56], extraction of antioxidant compounds [57], biodiesel production [58], ultrasound-assisted extraction and polysaccharide bioactivity [59], extraction of phenolic compounds [60] and food processing [61]. However, understanding the distribution of AE in plant materials and the kinetic parameters involved in their extraction is relevant in selecting the appropriate mathematical design or model for process simulation [62]. Previous studies report the use of different mathematical models applied to AE extraction [63], describing the impact of process variables and heat and mass transfer mechanisms [64-66].

This manuscript aims to analyse the variables associated with the different mathematical models or designs that calculated EO extraction yield using the hydrodistillation method, with an overview that explains the physical phenomena associated with the EO extraction process.

Materials and Methods

The PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) the guidelines for reviewing and searching the literature were followed [67].

Search Strategy

The databases used to search for scientific articles were EBSCO, SciELO, ScienceDirect, and Scopus. The following keywords were used: "yield essential/oils mathematical/model", "yield essential/oils mathematical/model and hydro distillation" and "yield essentials/oils data/mining hidrodistillation", see Table 1. The results were exported in an Excel sheet.

Table 1: Search strategy

Search number	Search terms/combinations
#1	yield and "essential oils" and "mathematical model"
#2	yield and "essential oils" and "mathematical model" and hydro distillation
#3	yield and "essentials oils" and "data mining" and hidrodistillation

Selection of Studies

For the review, original full-text articles published in English up to April 2023 were considered. To improve the quality of the review, peer-reviewed articles were analyzed, and results published as conference abstracts, doctoral dissertations, and master's theses were excluded [68-69]. After the search strategy, the titles and abstracts were analyzed based on the inclusion and exclusion criteria to determine which research was relevant for the review. Then, the full-text articles were examined to verify if they met the inclusion criteria according to the study objective.

Inclusion Criteria

The eligibility of the scientific documents acquired was established to the extent that they met the following criteria:

- (1) They should be complete;
- (2) The design used in the study should be experimental;
- (3) They should be written in English;
- (4) They should estimate the yield of essential oil extraction using mathematical models and the hydrodistillation method.

Exclusion Criteria

The exclusion criteria were:

- 1) Duplicate articles;
- 2) Studies that are systematic reviews of the literature, narrative reviews, opinion articles, commentaries, or editorials;
- (3) Studies that used mathematical models to determine a dependent variable other than extraction yield;
- 3) Studies that used a different method of essential oil extraction.

Table 2 details the inclusion and exclusion criteria.

Data Extraction

The manuscripts that met the inclusion and exclusion criteria were selected collaboratively. For this purpose, two standard Excel spreadsheets were used: The first selected the studies, as it contained the results by search words in the four databases, analyzed the abstract of the manuscript, and posed the status of being considered or not. The second spreadsheet was composed of characteristics such as: title of the manuscript, year of the experiment, country, species, common name of the species, plant material used, variables influencing extraction yield and finally the design or mathematical model.

Table 2: Inclusion and exclusion criteria for study selection

Parameter	Inclusion Criteria	Exclusion criteria
Type of article	Full text	
Study design	Experimental	Systematic reviews, narrative reviews, opinion articles, commentaries, editorials
Language	English	No english
Exhibition	mathematical models, extraction performance	
Primary results	Calculation of essential oil extraction yield by hydrodistillation using mathematical models	

Results

Studies Included

The PRISMA flow chart summarizes the study selection process (Fig. 1). The search yielded 825 manuscripts; (172) were eliminated due to duplication. And one article eliminated for plagiarism, leaving 653 articles that have been analyzed by title and abstract, of which 10 that were eliminated were not scientific articles (8), the full text was not in English (2). A total of 643 full-text articles were considered for subsequent evaluation, following the exclusion and inclusion criteria. Of these, 10 that were eliminated employed another hydrodistillation technique, 45 did not estimate extraction yield using mathematical models, and 571 did not address the subject matter. The remaining 17 manuscripts were deemed suitable for both quantitative and qualitative analysis. [70-83, 50, 84, 85].

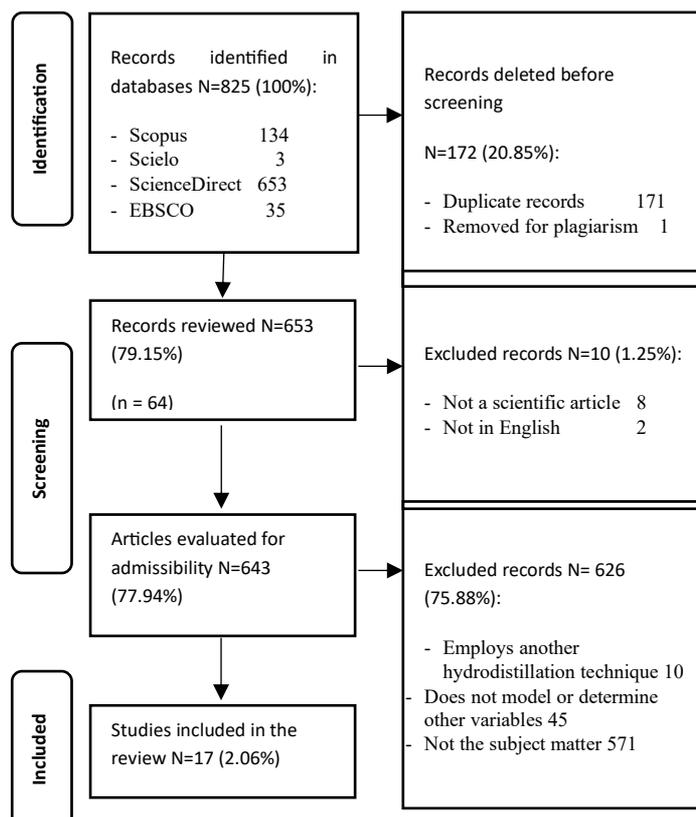


Fig. 1: Study selection process through PRISMA

Descriptive Characteristics of the Studies

Table 3 this shows a summary of the conditions present in the essential oil extraction yield estimation studies included. Of the seventeen articles considered, five were developed in Tunisia and Algeria belonging to Africa, five in Thailand, India, China and Vietnam in Asia, three in Mexico and Brazil in America, finally three in Serbia belonging to Europe. The total number of forest species studied was 19, where RSM was employed in ten manuscripts, kinetic models in four and data mining algorithms in three.

Discussion

Of the eight hundred and twenty-five (825) articles identified in the Scopus, ScienceDirect, Scielo and EBSCO databases (Fig. 1), duplicate records, those that calculated without the essential oil yield by mathematical modeling but not using the hydrodistillation technique, were eliminated [86-94], those who have used hydrodistillation to obtain the essential oil and thus compare it with other techniques [95-103]. Also manuscripts that established yield without resorting to mathematical models,

but whose estimated variable was plant material moisture, are included [104-107], total polyphenol content and radical scavenging activity [108], time required to detect the impact of essential oil in the evaluation [109], drying time, energy consumption, and quantity of essential oil [110], color parameters, color difference, humidity, essential oil content and eight main components identified [111].

Furthermore, the factors that affect the efficiency of EO extraction from the nineteen plant species have been categorized as agroclimatic elements (maximum and minimum average temperature, average rainfall, minimum and maximum relative humidity, and altitude, pH, organic carbon, nitrogen, phosphorus, potassium, sampling period), conditioning or pretreatment factors (particle size, swelling time, preparation time, drying time, milling time, drying air temperature, fruit fragmentation) and operating factors (distillation time, time after the first drop falls, solid/liquid ratio, condensation flow, hydrodistillation rate, mass ratios, temperature). The three plant materials most used by hydrodistillation were ten leaves, three fruits and two seeds. The findings corroborate that yield is affected by environmental factors, such as the material's moisture content, its origin, and the time of collection [112-113].

The advantage of hydrodistillation is its low cost and simplicity [114]. However, it has limitations, as it may not be suitable for some plant materials, especially those that are sensitive to heat, and may cause degradation of some of the more volatile components of the EO. In addition, it can be a slow process, some EOs require several hours of distillation [115]; since a shorter time can save energy and other resource costs for producers and processors [116].

Data mining and statistical analysis have been widely used to solve problems, especially in engineering, during the digital age [117]. The experimental designs most frequently used when applying RSM were the factorial design four times and the central composite design with Box-Behnken twice, respectively. Among the advantages of Data Mining (DM) is the applicability of an adequate knowledge of the different types of algorithms used, since they provide the same results, each one with a different efficiency [118]. Three selected papers have employed DM to estimate the extraction yield of essential oils, using nine algorithms, see rows 15, 16 and 17 of Table 3. Confirming that the use of technology is constantly growing, which has a significant effect in almost every field [119].

Table 3: Summary of studies included in the systematic review

Country	Species	Plant material	Variables	Experimental design or model	Percentage yield (%) /Extraction method	Model Evaluation (statistics)	Ref
Serbia	<i>Mentha piperita</i> L.	sheet	Extraction time (2.5, 5, 7.5, 10, 15, 30, 45, 60, 90, 120 min)	Kinetic model	0.73 / HD 0.80 / MAHD	$R^2 = 0.971$ to 0.981	[83]
Algeria	<i>Pimpinella anisum</i>	seed	Extraction time (5, 10, 15, 20, 40, 55, 70, 80, 90, 110, 130 min)	Kinetic model	3.30±0.05 / HD 2.81±0.01 / MAHD	$R^2 = 0.938$ and 0.968 / $R^2 = 0.979$	[82]
Tunisia	<i>Rosmarinus officinalis</i> var. <i>typicus</i> L.	sheet	Extraction time (0, 15, 30, 45, 60, 75, 90, 105, 120, 135, 150, 165 min)	Kinetic model	NS /HD	$R^2 = 0.93$	[80]
--	<i>Pimpinella anisum</i> , <i>Eucalyptus cinerea</i>	seed, sheet	Extraction time (0-15, 15-30, 30-60, 60-90, 90-120, 120-180, 180-240, 240-300, 300-360 min)	Kinetic model	1.28–4.01; 0.9– 2.20 /HD	$R > 0.98$	[71]
Thailand	<i>Fagraea fragrans</i> Roxb.	flower	Proportion of water and plant material (2.34, 4, 8, 12, 13.66). Extraction time (95, 15, 120, 180, 240, 264.85 min)	Central Composite Design/Response Surface Methodology	0.35±0.02 / HD	$R^2 = 0.880$	[6]
Vietnam	<i>Citrus reticulata</i> Blanco	shell	Proportion of water and plant material (2.32, 3, 4, 5, 5.68). Temperature (70, 90, 120, 150, 170 °C).	Central Composite Design/Response Surface Methodology	0,35±0,02 / HD	$R^2 = 0.970$	[84]

Tunisia	<i>Myrtus communis</i> L.	sheet	Extraction time (103, 110, 120, 130, 137 min). Time after the first drop of extraction (150, 180, 210 min). Condensation flow (0.2, 1.2, 2.2 ml/min). Plant material/water ratio (1/8, 1/6, 1/4). Granulometry ([0.5:1], [1;1.5], [1.5;2] mm).	Factorial design/response surface methodology	0.635 / HD	$R^2 = 0.923$	[70]
Tunisia	<i>Thymus algeriensis</i> Boiss. & Reut	sheet	Extraction time (120, 240 min). Temperature (250, 350 °C). Ratio of plant material to water (0.125, 0.25). Sampling period (flowering, fruiting).	Factorial design/response surface methodology	0.223 - 1.428 / HD	$R^2 = 0.999$	[85]
Mexico	<i>Eucalyptus urograndis</i>	sheet	Plant mass/water ratio (1:1, 1:3, 1:5 g/mL).	Factorial design/response surface methodology	1.19±0.01 / HD	$R^2 > 0.90$	[50]
Brazil	<i>Schinus terebinthifolius</i> Raddi	fruit	Drying air temperature (50, 60, 70 °C). Types of fruit fragmentation prior to essential oil extraction (whole dried and fragmented in a blade mill after drying).	Factorial design/linear regression	2.4–2.9 / HD	$R^2 > 0.99$	[81]
China	<i>Carex meyeriana</i> Kunth	sheet	Water/plant material ratio (30:1, 40:1, 50:1 mL/g). Extraction time (7, 9, 11 h). Mesh particle size (0, 10, 20).	Design Box-Behnken / response surface methodology.	0.13 / HD	$R^2 = 0.96$	[79]
China	<i>Cirsium japonicum</i> Fish ex DC, <i>Cirsium setosum</i> (Willd.) M.Bieb	sheet	Soaking time <i>japonicum</i> (3, 6, 9 h). <i>Setosum</i> (1, 3, 6 h). Proportion of water and plant material <i>japonicum</i> (15, 20, 25). Proportion of water and plant material <i>Setosum</i> (10, 15, 20). Extraction time <i>japonicum</i> (120, 140, 160 min). Extraction time <i>Setosum</i> (3, 5, 7 h).	Box-Behnken Design / response surface methodology.	0,0582±0,0015/HD 0,0383±0,0010 / HD	$R^2 = 0.999$	[73]
Serbia	<i>Juniper berries</i>	fruit	Grinding time (1, 2, 3 min). Swelling time in distilled water (24, 48, 72 h).	Experimental design/response surface methodology	2.23±0.00 / HD	$R^2 = 0.805$, $R^2_{adj} = 0.775$	[78]

Brazil	<i>Pinus taeda</i> L.	sheet	Quantity of biomass (20, 30, 40 g). Extraction time (1, 1.5, 2 h). Sample size (2, 3, 4 cm). Drying time (24, 48, 72 h).	Box full factorial design/response surface methodology	0.25-0.53 / HD	$R^2 = 0.968$, $R^2_{adj} = 0.856$	[74]
India	<i>Curcuma longa</i> L.	root	Maximum and minimum relative humidity. Average rainfall. Maximum and minimum average temperature. Altitude. pH. Organic carbon. Nitrogen. Phosphorus. Potassium.	Artificial Neural Networks	0.8-1.2 / HD	$R^2 = 0.88$	[77]
Algeria	<i>Marrubium vulgare</i> L.	entire plant	Mass radii (3, 5, 7 kgm ⁻³). Particle size (d>2, 1.25<d<2, 0.63<d<1.25, 0.1<d<0.63 mm).	Evolutionary algorithms. Genetic algorithm. Particle swarm optimization	7.19-19.65 / HD	0.995<R<0.998	[75]
Serbia	<i>Juniperus communis</i> L.	fruit	Swelling time (h). Preparation time (min). Hydromodule. Hydrodistillation rate (ml/cm ³). Essential oil yield (%). Altitude (meters above sea level). Measured quantities of essential oil separated in X minutes (5, 10, 15, 20, 25, 30).	Decision Tree, Random Forest, k Nearest Neighbors, Support Vector Machines, Naïve Bayes Classifier.	1.09-2.49 / HD	NS	[76]

Note. HD: Hydrodistillation, MAHD: Microwave-assisted hidrodistillation, NS: Not specified

The variable in the estimation using the kinetic model of essential oil obtaining yield was time, which yielded diverse results due to factors such as the species and component of the plant under study, see Table 3 from row one to row four. In addition, the models had a coefficient of determination between 0.930 and 0.981, indicating an excellent fit of the model, capturing most of the relationship between the variables. On the other hand, the designs used in the response surface methodology were Central Composite Design, Factorial design, Box-Behnken design, Experimental design, and Box full factorial design, where the variables extraction time and ratio of plant material to water were used in more than 50% of the research that has employed this modelling technique. However, the R2 closest to one was obtained in the Box-Behnken design, see lines five to fourteen of Table 3. Unlike the two previous modelling approaches, DM algorithms (Decision Tree, Random Forest, k Nearest Neighbors, Support Vector Machines, Naïve Bayes Classifier, Artificial Neural Networks, etc.) can work with multiple variables defined in the reviewed studies, see lines fifteen to seventeen, and the values of R2 were greater than 0.88.

The variable used in estimating essential oil yield using the kinetic model was time, which yielded different results due to factors such as the plant species and component studied (see Table 3, rows one to four). Furthermore, the models exhibited a coefficient of determination between 0.930 and 0.981, indicating an excellent fit and capture of most of the relationship between the variables. The designs used in the response surface methodology were the Central Composite Design, the Factorial Design, the Box-Behnken Design, the Experimental Design, and the Full Box-Behnken Factorial Design. The variables of harvest time and the ratio of plant material to water were used in more than 50% of the studies that employed this modeling technique.

Conclusion

Mathematical models and Data Mining (DM) algorithms are used to estimate the distillation yield of essential oils (EO) by hydrodistillation. The literature showed that work has been carried out in Americas, Europe, Asia, and Africa; considering 18 plant species and leaves being the most frequently used plant material in hydro distillation extraction. The mathematical models used were kinetic, response surface and DM algorithms, with the input variables being agro-climatic, pre-treatment or conditioning and operating variables.

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Author's Contributions

Lenin Quiñones Huatangari: Conducted the literature search and data extraction and authored the initial draft of the manuscript.

Frank Fernandez Rosillo: Authored the initial draft of the manuscript.

Eliana Milagros Cabrejos Barrios, Erika Guisella Quinde Flores and María Alina Cueva Ríos: Prepared the manuscript for publication.

Elza Berta Aguirre Vargas: Critically reviewed and provided substantial edits to the manuscript.

Ethics

This article presents previously unpublished material. The lead author confirms that the manuscript has been read and approved by the other authors and confirms that there are no ethical concerns.

Conflicts of Interest

The authors claim to have no conflict of interest.

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