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MULTI-OBJECTIVE OPTIMIZATION OF THE GREEN EXTRACTION CONDITIONS OF BIO-ACTIVE COMPOUNDS FROM A *LEVISTICUM OFFICINALE* WDJ KOCH: PARETO OPTIMALITY AND COMPROMISE SOLUTIONS FOR PROCESS MANAGEMENT

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ABSTRACT

Plants belonging to the Apiaceae family (including *Levisticum officinale* WDJ Koch) are rich sources of phytochemicals and secondary metabolites, with possible health-promoting and agrochemical potential. The objective of this work was to provide important guidelines for controlling conventional aqueous extraction to obtain *Levisticum officinale* root extracts with maximised levels of bioactive compounds. The ultimate goal was to optimise the total phenolic compounds, flavonoid content, sugars, and total antioxidant capacity to identify the process conditions necessary to produce highly bioactive extracts that could be used in a wide range of industries. Biomass extraction of lovage root was carried out using water as the extraction solvent. To perform the optimisation of the aqueous extraction, multivariate regression models were used and multi-criteria analysis was performed using Pareto set navigation. Pareto front analysis showed that for the maximum extraction efficiency of bioactive compounds from *Levisticum officinale*, the optimal extraction process parameters were 0.0714 $g \cdot mL^{-1}$ as biomass/water ratio and a time of 35.7142 min, at the highest analysed temperature. For the highest analysed value of plant biomass/solvent ratio (0.075 $g \cdot mL^{-1}$) and maximum process temperature (95ºC), extraction could be carried out for 20 min or in the range 37.1429-38.5714 min. On the other hand, if the extraction time reaches 40 min and the sam-ple/solvent ratio 0.075 $g \cdot mL^{-1}$, the optimum process temperature is be-tween 75ºC and 95ºC.

Introduction

The centuries-old tradition of using aromatic plants in folk medicine has become part of the current search for new agricultural, food, pharmaceutical, or cosmetic products. Previous research has shown that plants belonging to the Apiaceae family (including *Levisticum officinale* WDJ Koch) are a rich source of phytochemicals and secondary metabolites, with possible health-promoting and agrochemical potential (Aćimović et al., 2015; 2.Tunçtürk and Özgökçe, 2015; Spréa et al., 2020). Research into the production of plant extracts with antioxidant potential, using diverse extraction methods, is a current research trend, in terms of their use in food production and sustainable agriculture (Szparaga, 2023a; Szparaga, 2023 b). Particular attention is currently focused on the optimisation of production processes in terms of extraction parameters for maximising antioxidant levels (Lee et al., 2013; Radojković et al., 2012; Vuong et al., 2011; Algan Cavuldak et al., 2019). Antioxidant compounds (including polyphenols and flavonoids) are a widely distributed group in the plant kingdom. The potential of bioactive compounds is used in medicine, and not only in the effective treatment of many chronic diseases (Özcan et al., 2018) but also in the prevention of oxidative stress damage and diseases of civilisation (Mahdi et al., 2019), as well as in agronomy, due to the fact that they are involved in the stimulation of plant growth, as well as in plant responses to environmental stresses (Chalker-Scott and Fuchigami, 2018). Their antioxidant potential is also a promising property for enhancing the tolerance of crop plants to changing climatic conditions, in the aspect of not only phytoprotective but also biostimulatory effects (Parvin et al., 2022). Therefore, the scientific basis for understanding effective extraction methods and optimising antioxidant activity, is important for the use of natural plant extracts in the food or pharmaceutical industry, as well in large-scale agro-industrial systems (Melo et al., 2015). Nowadays is a growing trend in research into natural antioxidant compounds that could replace synthetic products, including food additives and agrochemicals, commonly used in food production and agriculture (Kaur et al., 2006). Extracts from plant materials, rich in phenolic compounds, are becoming of increasing interest in organic farming, as they may show biostimulant, antifungal and bioprotective potential (Shukla et al., 2009). In the search for plant biomaterials for various applications, attention is being paid to conventional methods, based on solid-liquid extraction using water, considering the ecological aspect of this process. The rationale behind this approach includes eliminating undesirable effects on the environment, as well as on people and crops (Gil-Ramírez et al., 2012; Ahmadian-Kouchaksaraie et al., 2016). However, for the optimisation of aqueous bioextraction, it is important to consider the main parameters such as process temperature, solid/liquid ratio, and extraction time (Vuong et al., 2011), which will determine the potential and utilisation of the produced extracts (Murugesh et al., 2018). Therefore, given the negative impact of chemical processes and current aspirations and legislation (including the objectives and principles of Green Chemistry and the European Green Deal), sustainable and environmentally friendly solutions are being sought, including optimization of production processes, to increase extraction efficiency while eliminating immediate and long-term environmental impacts (Martiny et al., 2021). Considering the above aspects, the current tendency is to promote bioproducts, including plant extracts, as valuable tools with pharmacological potential, as well as biostimulatory for crops (Gonçalves, 2021; Dastan et al., 2022). The extraction process is considered an operation to produce bioactive materials from biological matrices (Chouhan et

al., 2019). Conventional extraction methods include maceration, Soxhlet extraction, or hydrodistillation. Nevertheless, many researchers have underlined that organic solvents are too commonly used in these methods (Dastan et al., 2022; Farahmandfar et al., 2019). Currently, water has become increasingly important as an environmentally friendly extraction solvent, with properties that can be controlled by changing temperature (Ahmadian-Kouchaksaraie et al., 2016). However, according to Batinić et al. (2022), it is difficult to develop a general protocol for the extraction of active compounds, including phenolic compounds, from plant materials, therefore the extraction process should be optimised for each source of plant material (Batinić et al., 2022). Green extraction operations should be integrated with efficient optimisation methods with a view to specifying the effectiveness of extraction techniques, such as Multi-objective optimisation, Multicriteria decision analysis (Mahdi et al., 2019; Bystrzanowska and Tobiszewski, 2019). Multivariate optimisation is currently gaining increasing importance in process design, where modelling, optimisation of results, and their scaling to industrial production, is carried out for several variables with multiple responses simultaneously.

In light of the above, this research aims to provide some important guidelines for controlling conventional aqueous extraction to obtain *Levisticum officinale* root extracts with maximised levels of bioactive compounds. Therefore, the present study evaluated and optimised the antioxidant potential of aqueous extracts from *Levisticum officinale* in terms of analysing the influence of extraction process parameters, i.e. temperature, time, and plant biomass/solvent ratio. The final objective was to optimise the total phenolic compounds, flavonoid content, sugars, and total antioxidant capacity for identifying the process conditions necessary to produce highly bioactive extracts that could be used in a wide range of industries. It can be expected that innovations in the use of decision theory based on mathematical models and broad optimisation tools, with the objective of improving and optimising conventional extraction techniques, can provide a new and broader dimension for increasing research opportunities in Multi-objective optimisation of ecological extraction methods.

Material and Methods

Plant material

The dried roots of an organically grown *Levisticum officinale* (sourced from Runo Polska, PL-EKO 07 EU Organic Farming) were ground to powder (fraction size of 500 μm). The ground powder was stored at 4ºC in airtight bags until further use.

Hot water extraction (HWE)

Extraction using lovage root biomass was carried out with 100 ml of water (at pH 7.0) as an extraction solvent. Extraction was carried out in an Elpin + type 357 shaking water bath. For HWE, the independent variables were extraction time (20, 30, and 40 min), temperature (75, 85, and 95ºC), and plant biomass/water (w/v) ratio (0.025 $g \cdot mL^{-1}$, 0.050 $g \cdot mL^{-1}$ and 0.075 $g \cdot mL^{-1}$). All extractions were carried out in triplicate. Extractions were followed by centrifugation (9500 rpm, 20 min) and filtration (Whatman® No. 1 filter paper). The collected supernant was stored at 4ºC in sealed dark glass bottles until further use.

Bioactive characterization of obtained extracts

In the extract, the total phenolic content (TPC) was determined. Quantification of total phenolic compounds was carried out using a modified method proposed by Ribeiro et al. (2008). A calibration curve was made using gallic acid as a standard and the polyphenol content was determined in mg gallic acid·g^{-1} extract.

The total flavonoid content (TFC) of the extracts was determined by the method proposed by (Iqbal et al., 2012). The TFC content in the samples was calculated as catechin equivalent (μmol·L^{-1}) from a standard catechin standard curve.

The total antioxidant activity (TAA) was also assessed in the extracts. The antioxidant activity of DPPH (2,2-diphenyl-1-picrylhydrazyl) was determined according to the method of Lee et al. (2013). The scavenging activity was calculated according to Equation:

$$\text{Scavenging activity } (\%) = [(\text{Abs}_{\text{control}} - \text{Abs}_{\text{sample}})/\text{Abs}_{\text{control}}] \text{ x } 100 \quad (1)$$

The content of reducing sugars (RSC) was determined using the 3,5-dinitrosalicylic acid (DNSA) method. The measurement was carried out according to the procedure by Krivorotova and Sereikaite (2014). The amount of reducing sugars in the extracts was calculated using a standard curve for D-glucose and the results were expressed as g of D-glucose equivalent (GE) per L of extract.

Mathematical model

The strategy to improve the extraction efficiency, in terms of increasing the level of bioactive compounds, was to use mathematical models and optimisation tools using computer calculation and simulation packages. The application of optimization techniques to the solution of specific agro-food problems, is now highly valued, as it allows efficient and intelligent support for the design of unit processes, enabling the production of a highly acceptable product. Therein this approach fits in the current research, among others, in the field of decision-making theory based on mathematical models and optimization results.

Multivariate regression models (Matlab R, 2021a) were used to perform the optimisation of the aqueous extraction. The models were derived from experimental data and quality characteristics of extracts from *Levisticum officinale*. The analysed process parameters/decision variables were sample/solvent ratio (g·mL^{-1}) (x_1), time of extraction (min) (x_2), and temperature of the extraction (ºC) (x_3).

The dependencies of the selected decision criteria on the decision variables were described using multivariate polynomials, defined as:

$$y_{reg}(x_1, x_2, x_3) = a_0 + a_1 * x_1 + a_2 * x_2 + a_3 * x_3 + a_4 * x_1 * x_2 + a_5 * x_1 * x_3 + a_6 * x_2 * x_3 + a_7 * x_1^2 + a_8 * x_2^2 + a_9 * x_3^2 \quad (2)$$

The quality of fit of the model to the experimental data was evaluated based on the obtained values of the R^2 Statistic, adjusted R^2 (Adj R^2), and Mean Squared Prediction Error (MSE) indices (Curve fitting, 2004).

R^2 as a statistic measures the effectiveness of the fit in explaining variation in the data. Mathematically, it is the square of the correlation between response values and predicted response values. R^2 is also the square of the multiple correlation coefficient and the multiple determination coefficient. In notation, it is defined as the ratio of the sum of squares of the regression (SSR) and the total sum of squares (SST) (Curve fitting, 2004). SSR is defined as

$$SSR = \sum_{i=1}^{n} w_i \, (\hat{y}_i - \bar{y})^2 \tag{3}$$

SST is also called the sum of squares around the mean and is defined as:

$$SST = \sum_{i=1}^{n} w_i \, (y_i - \bar{y})^2 \tag{4}$$

where:

$$\text{SST} = \text{SSR} + \text{SSE} \tag{5}$$

Given these definitions, the R^2 is expressed as

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST} \tag{6}$$

The R^2 coefficient can take any value from 0 to 1, with a value closer to 1 indicating a higher degree (higher measure) of fit.

The adjusted R^2 statistic is generally the best indicator of the quality of fit when additional coefficients are added to the model.

$$Adj\ R^2 = 1 - \frac{SSE(n-1)}{SST(v)} \tag{7}$$

where:

v – Degrees of Freedom,

SSE – Sum of Squares Due to Error,

SST – the sum of squares about the mean.

$$SSE = \sum_{i=1}^{n} w_i (y_i - \widehat{y_i})^2 \tag{8}$$

SSE is a statistic that measures the total deviation of the response value from the match to the response value.

The adjusted R^2 statistic can take any value less than or equal to 1, with a value closer to 1 indicating a higher degree (higher measure) of fit (Curve fitting, 2004).

Mean Squared Prediction Error (MSE) measures the mean squared deviation between the experimental data and theomi values derived from the adopted model:

$$MSE = \frac{SSE}{v} \tag{9}$$

Multi-objective optimization

In the optimization task under consideration, a four-dimensional criteria space was assumed $K = [K_1, K_2, K_3, K_4] \in R^4$, in which solutions were sought for which all criteria would take extreme values. The multi-objective extraction optimization procedure is shown in Figure 1.

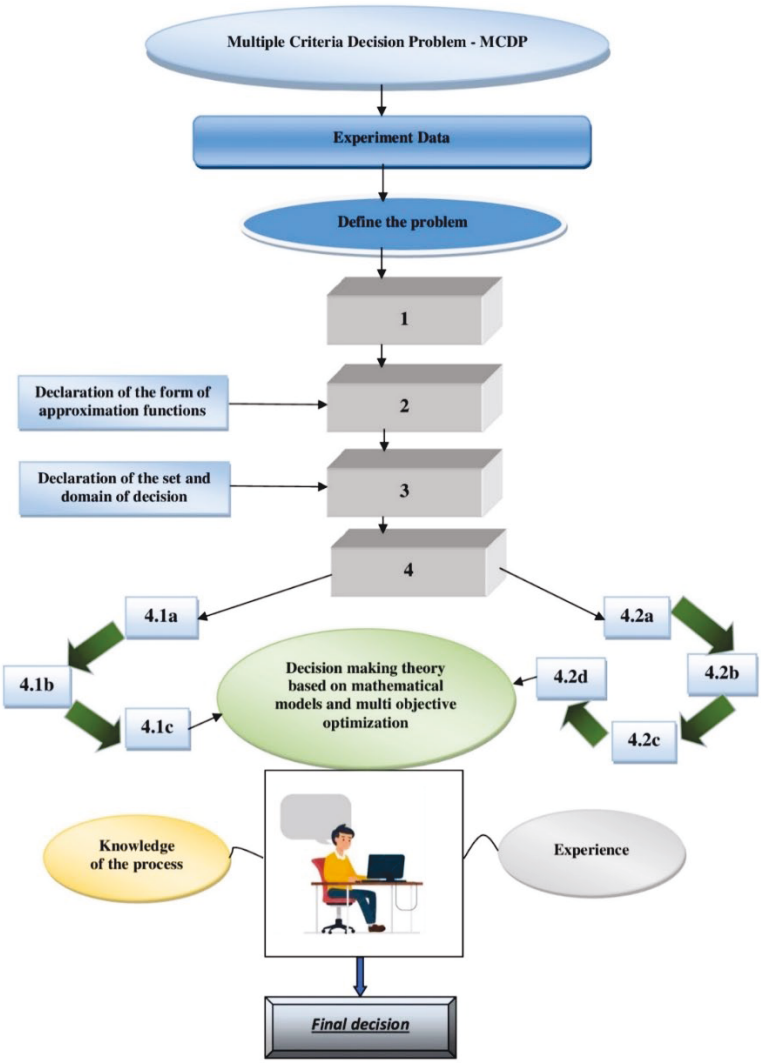

Figure 1. The flowchart of Multi-objective optimization of the extraction
Legend: 1 – Uploading experimental data; 2 – Mathematical Model – Multidimensional Regression; 3 –Determination of the value of the decision criteria; 4 – Normalization of the decision criteria; 4.2a – Calculation of the distance from the Utopia solution in the space of decision criteria; 4.2b – Determine a boundary value of metric for compromise solutions; 4.2c – Determination of the metric value for the analyzed set of solutions in the decision criteria space; 4.2d – Determination of sets of compromise solutions in decision variables; 4.1a –Determination of sets of dominated and Pareto-optimal solutions in the space of decision criteria; 4.1b –Determination of the Pareto front in the space of decision criteria and variables; 4.1c – Determination of a subset of Pareto-optimal solutions in the space of decision variables

The goal of the optimization was to obtain an aqueous extract from *Levisticum officinale*, characterized by the maximum value of criteria K_1-K_4. Decision criteria were defined in the following forms:

– Criterion K_1 – TPC total phenolic content, (mg GAE·g^{-1})
– Criterion K_2 – TFC total flavonoids content, (μmol CAT·L^{-1})
– Criterion K_3 – TAA total antioxidant activity, (DPPH-%inh)
– Criterion K_4 – RSC reducing sugar content, (g GE·L^{-1})

The criteria were calculated for a defined set of decision variables for the extraction process:

– Decision variable x_1 – Sample/solvent ratio, (g·mL^{-1})
– Decision variable x_2 – Time, (min)
– Decision variable x_3 – Temperature, (ºC)

The mathematical form of the set of decision variables (domain) was defined by the formula:

$$D = x_1 \times x_2 \times x_3 \tag{10}$$

Constraints imposed on decision variables:

$$x_1 \in \langle 0{,}025\ ;\ 0{,}075 \rangle\ (g \cdot mL^{-1}) \tag{11}$$

$$x_2 \in \langle 20\ ;\ 40 \rangle\ (min) \tag{12}$$

$$x_3 \in \langle 75\ ;\ 95 \rangle\ (^{\circ}C) \tag{13}$$

The values of all decision criteria for a fixed set of decision variables D were determined by multivariate approximation of experimental results.

Multi-objective optimization task consisted in determining the set of solutions in the set D for decision criteria satisfying conditions:

$$K_1 \rightarrow max, K_2 \rightarrow max, K_3 \rightarrow max, K_4 \rightarrow max$$

To facilitate the solution of this task, the decision criteria were scaled to dimensionless variables and normalized as follows:

$$K_i^{(n)} = \frac{K_i^{max} - K_i}{K_i^{max} - K_i^{min}}\ i = 1{,}2{,}3{,}4\ k_i^{(n)} \in \langle 0; 1 \rangle \tag{14}$$

where:

K_i^{min} i K_i^{max} denote the smallest and largest value of the criteria, respectively, for the analyzed set of decision variables D.

The normalization procedure made it possible to compare with each other the values of criteria describing different quantities and expressed in different units. The maximum value of the actual criterion corresponds in the space of normalized criteria to the value of 0. In the following part of the procedure, only normalized decision criteria will be used with the superscript (n) at K omitted. In the next step, a dominance relation was introduced between two, arbitrary vectors of decision criteria *K*=[K_1, K_2, K_3, K_4] and K'=[K_1', K_2', K_3',K_4'] belonging to the set *D* of the form:

$$K \succ K' \Leftrightarrow K - K' \in C \quad C = \{(a_1; a_2; a_3; a_4) \in R^4 : a_1, a_2, a_{3,}, a_4 \leq 0\} \qquad (15)$$

If one assumes that the K=[K_1, K_2, K_3, K_4] will be any vector in the space of decision criteria, then the solution X^* is called optimal in the Pareto sense if the implication is true for any admissible solution X:$K(X^*) \succ K(X) \Rightarrow K(X^*) = K(X)$.

The set of all possible Pareto-optimal solutions is also called the set of non-dominated (Pareto-optimal) solutions. On this basis, the explicit form of the set of dominated and non-dominated (Pareto-optimal) solutions for water extracts in the space of decision criteria was determined. The set of Pareto-optimal and dominated solutions form a set in a four-dimensional criteria space. To analyze and visualize these sets, subsets of the four-dimensional space (K_1, K_2, K_3, K_4) in three-dimensional and two-dimensional decision criteria spaces were considered (Gómez-Salazar et al., 2022).

Reduce the Set of Pareto Optimal Solutions – the compromise solutions

By definition, Pareto optimal solutions are incomparable with each other. Therefore, to select a smaller subset from the set of these solutions, a reduction of this set can be carried out by applying an efficiency measure for each element of the Pareto set. In the optimization task, the definition of the Utopia point considered the optimal solution in all respects (efficiency of order 1), is adopted (Szparaga et al., 2019; Sato at al., 2017). The Utopia point is the ideal point that maximizes the goals simultaneously (the so-called unattainable point). Therefore, the concept of achievable preferred solutions on the Pareto front with a minimum distance from the Utopia point (d_U) was introduced (Fig. 2). To find this compromise solution on the Pareto front, first the objective functions were normalized to the range [0,1].

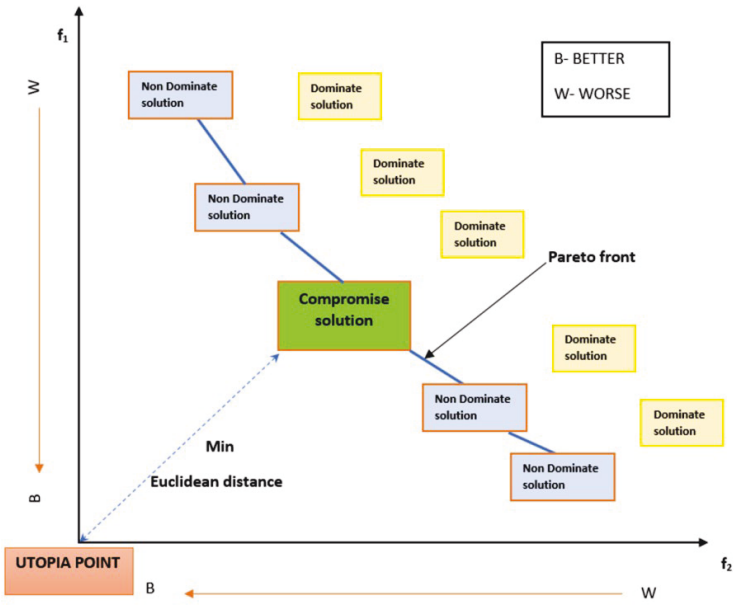

Figure 2. Scheme for determining the set of compromise solutions from the Pareto front

Then the Euclidean distance of all solutions on the Pareto front, measured from the Utopia point, was determined. The Pareto-optimal solution with the minimum distance from the Utopia point was selected as the best solution from the given set (Foroughi and Razavi, 2022).

Thus, to analyze the set of all admissible solutions, a Euclidean metric of the form was introduced in the space of normalized decision criteria:

$$d_U = d(K_0\, K) = \sqrt{\sum_{i=1}^{4} K_i^2} \qquad \ldots(16)$$

where:

K_0=(*0, 0, 0, 0*) is the origin of the coordinate system, the so-called utopian solution (d_U).

The obtained solutions can be regarded as the best solutions from the obtained Pareto set in terms of equal satisfaction of all criteria.

Statistical analysis

An analysis was carried out in Matlab using the F-statistic for testing the statistical significance of the model. The values of the F-statistic for testing the final model vs. no model (mean only) allowed us to assess the significance of the elements or components of the model (Curve fitting, 2004). The sse - sum of errors squared (residuals), specified as a numerical value, was given. The ssr was also determined - the sum of squares due to regression or explained sum of squares (ESS) is the sum of the differences between the predicted value and the mean of the dependent variable and p*val* - a vector of *p*-values for testing whether elements of b are 0.

Results and Discussion

For the adopted model in the form of polynomials of many variables, the coefficients of the equation were determined (Table 1).

The model allows the decision variables (process parameters) to be optimised for maximum response, in this case, the yield of phenolic compounds (TPC). The effectiveness of the model can be represented by R^2, Adj R^2, and MSE values. The results of the analysis (Table 1) show the predictive ability of the model for TPC. The R^2 value for the total phenolic content was 0.858, which means that the model explains about 85% of the variation in responses. The adjusted R^2, which is always less than or equal to R^2, took on a value of 0.783. The similar values of both indices (difference of 0.075) indicate that the model, predicts the values in the target field, very well. i.e. has predictive value.

The R^2 value for criterion 2, i.e. total flavonoid content (TFC), was 0.905, meaning that the model satisfactorily described the actual relationships between the selected decision variables. The adjusted R^2 value (Adj R^2) in the model (0.855) was close to R^2 (with a difference of 0.050). The coefficients determined indicate that their values were close to 1, indicating a high degree of correlation between the experimental values and those predicted by the model.

Table 1.
Regression equations and indicators of model fitting to experimental data for the decision criteria

Criteria	Model			
TPC	$TPC = 725.247 + 13272.872x_1 - 9.908x_2 - 18.966x_3 + 20.22x_1x_2 - 65.583x_1x_3 + 0.009x_2x_3 - 52896x_1^2 + 0.157x_2^2 + 0.141x_3^2$	MSE	R^2	Adj R^2
		121.539	0.858	0.783
	Parameters of model performance evaluation	sse	2.07e+04	
		F-value	11.4314	
		ssr	1.25e+05	
		p-value	1.32e-05	
TFC	$TFC = 3338.421 + 27965.5x_1 + 8.709x_2 - 94.049x_3 + 131.9x_1x_2 - 127.34x_1x_3 - 0.08x_2x_3 - 141485x_1^2 - 0.1485x_2^2 + 0.642x_3^2$	MSE	R^2	Adj R^2
		40.384	0.905	0.855
	Parameters of model performance evaluation	sse	7.49e+04	
		F-value	17.968	
		ssr	7.12e+05	
		p-value	5.23e-07	
TAA	$TAA = 131.179 - 9.1x_1 - 0.178x_2 - 1.662x_3 + 0.943x_1x_2 + 0.653x_1x_3 - 0.002x_2x_3 + 4.444x_1^2 + 0.0049x_2^2 + 0.011x_3^2$	MSE	R^2	Adj R^2
		0.886	0.855	0.778
	Paremeters of model performance evaluation	sse	15.062	
		F-value	11.1425	
		ssr	88.852	
		p-value	1.58e-05	
RSC	$RSC = 6.09 + 653.233x_1 - 0.231x_2 - 0.366x_3 + 8.573x_1x_2 - 4.18x_1x_3 - 0.007x_2x_3 - 2720.9x_1^2 + 0.0063x_2^2 + 0.0049x_3^2$	MSE	R^2	Adj R^2
		13.187	0.817	0.721
	Paremeters of model performance evaluation	sse	224.183	
		F-value	8.433	
		ssr	1.00e+03	
		p-value	9.95e-05	

Legend: sse - The sum of errors squared (residuals), defined as a numerical value; ssr - The sum of squares due to regression - the sum of the differences between the predicted value and the mean of the dependent variable, *p*val - A vector of *p*-values for testing whether elements of b are 0; *F*-value - F statistic.

The situation for TAA (total antioxidant activity) was similar to the fit between experimental and predicted data. The R^2 coefficient took a value of 0.886 and the adjusted R^2 was 0.778. The responses had a difference between the predicted R^2 and the adjusted R^2 of 0.077, which was considered sufficient to explain the variability in responses (model fit). Fitting the model to the experimental data for reducing sugar content (RSC) indicated that the model was well suited for prediction. The correlation coefficient was 0.817, while its adjusted value was 0.721. According to Song et al. (2011), the regression coefficient represents the strength of the model's representation of the experimental data, while the *p*-value is a useful tool for checking the significance of the correlation (Song et al., 2011). In addition, an important aspect is the determination of the MSE (checking how close the predicted values are to the

actual values), the sum of squared differences between predicted data and the mean of the response variable (ssr), and the sum of squares error (sse) i.e. the sum of squared differences between predicted data and observed data points. The values of the indicators are shown in Table 1 for each criterion. The smallest value of mean squared error was recorded for TAA and RSC. The largest, however, was for TPC.

Based on experimental studies, it has been confirmed that extraction efficiency is determined by a number of different parameters, including the type of solvent, the method or technique, process time, temperature, or the sample-to-solvent mass ratio (Azwanida, 2015; Humadi and Istudor, 2009; Khatri and Chhetri, 2020). It should be emphasised that the appropriate extraction technique and choice of solvent are not only important in terms of extracting biologically active compounds from plant biomass but are also ecologically relevant. Based on the above, water was chosen for this study as a neutral solvent in the heat-assisted extraction process. The quantification of total phenolic compounds (TPC) showed that all analysed variables influenced this parameter. Depending on the temperature, time, and also the ratio of plant biomass to solvent used in the extraction, different extraction efficiencies of these compounds were observed. Of all the extract samples tested, the TPC was highest for extracts from *Levisticum officinale*, extracted at the analysed maximum temperature (95ºC) with a 40 and 20 min process time at a plant biomass/water ratio of 0.075 $g \cdot mL^{-1}$. Similar TPC contents were recorded for extracts produced at 85ºC and for 30 min. The lowest levels of these bioactive compounds were observed at the lowest plant biomass/solvent ratio analysed (0.025 $g \cdot mL^{-1}$). In the case of TPC, their lowest concentration was the result of using the shortest 20-minute extraction time and a process temperature of 85ºC. It was also found that, for samples extracted at the lowest plant biomass/water ratio, increasing the extraction temperature to 95ºC and increasing the process time resulted in an increase in the total pool of phenolic compounds. Similar trends were observed for the other process factor combinations tested. However, increasing the root biomass ratio of *Levicum officinale* from 0.050 to 0.075 $g \cdot mL^{-1}$ no longer resulted in significant increases in the extraction efficiency of phenolic compounds.

Studies on bioactive compounds in *Levisticum officinale* root extracts showed that the flavonoid concentration (TFC) was determined by the conditions of the extraction process. A lower TFC was the result of producing extracts at the lowest plant biomass/water ratio. Among all combinations analysed, samples extracted at 75ºC for 40 minutes had the lowest flavonoid pool. A twofold increase in the extraction efficiency of flavonoids from the biomass of *Levisticum officinale* root resulted from increasing the mass/volume ratio of plant material and water to 0.050 and 0.075 $g \cdot mL^{-1}$. Between the two groups, the variation in flavonoid levels was no longer as great. It was also found that increasing the process temperature to 95ºC, led to extracts more abundant in flavonoids. The highest TFC was recorded for extracts produced at a biomass/solvent ratio of 0.075 $g \cdot mL^{-1}$ and when an extraction temperature of 95ºC was used. The highest levels of antioxidant capacity were obtained at the highest plant biomass/solvent ratio regardless of the extraction temperatures and process times used. Admittedly, an increase in extraction temperature resulted in an increase in the tested response. Similar relationships were noted for the content of reducing sugars. In both cases, greater control of the process parameters for maximising the level of the characteristics tested was also noted.

The studies presented here are among the few that have used water as an extracting agent. However, it should be mentioned that currently, when selecting solvents, not only factors such as solubility, and selectivity, but also their safety, ecological dimension, and cost should be taken into account. This fits in with the basic goals and efforts underlying green chemistry, which are, among others, to reduce the use and production of hazardous chemicals in chemical processes, while optimising these processes to reduce their immediate and long-term environmental impact. Green chemistry guidelines have gained wide recognition as standards for assessing the environmental performance of a process (Martiny et al., 2021).

The experimental and modelling results are in agreement with those of Dastan et al. (2022). The authors found that both polyphenol, flavonoid content, and antioxidant potential were determined by the sample: solvent ratio. A study by Dixit et al. (2005) on the antioxidant properties of fenugreek seed extracts, found that the polyphenol and flavonoid content could be intensified by appropriate parameters using only water as a solvent. The effect of the biomass/solvent ratio is mainly due to the conversion of the plant matrix to the solvent. A solvent being at an equilibrium point can induce a reduction in the mass transfer of biomaterials into the extract (Dastan et al., 2022; Chemat and Cravotto, 2013). An additional factor that affects extraction efficiency is the process temperature. Sometimes higher process temperatures result in the release of a larger pool of phenolic compounds into the solvent and crude extract (Hayat et al., 2009). However, there are also findings in the literature that indicate that higher temperatures lead to reduced extraction efficiency due to the degradation of phenolic compounds (Singh et al., 2017). There is a belief that medium temperature ranges are considered 'optimal' (Singh et al., 2017; Vu et al., 2019).

The interpolation and regression functions of criterion K_1- K_4 as a function of process parameters (decision variables) are shown in Figures 3-6.

Figures 7-9 show Pareto fronts in the decision criteria space. To better visualise the effects of multi-objective optimisation, Figures show the Pareto solution sets for the maximisation of the regression equations as a function of the decision variables x_1 (Sample/solvent ratio), x_2 (Time) and x_3 (Temperature) in 2D and 3D spaces.

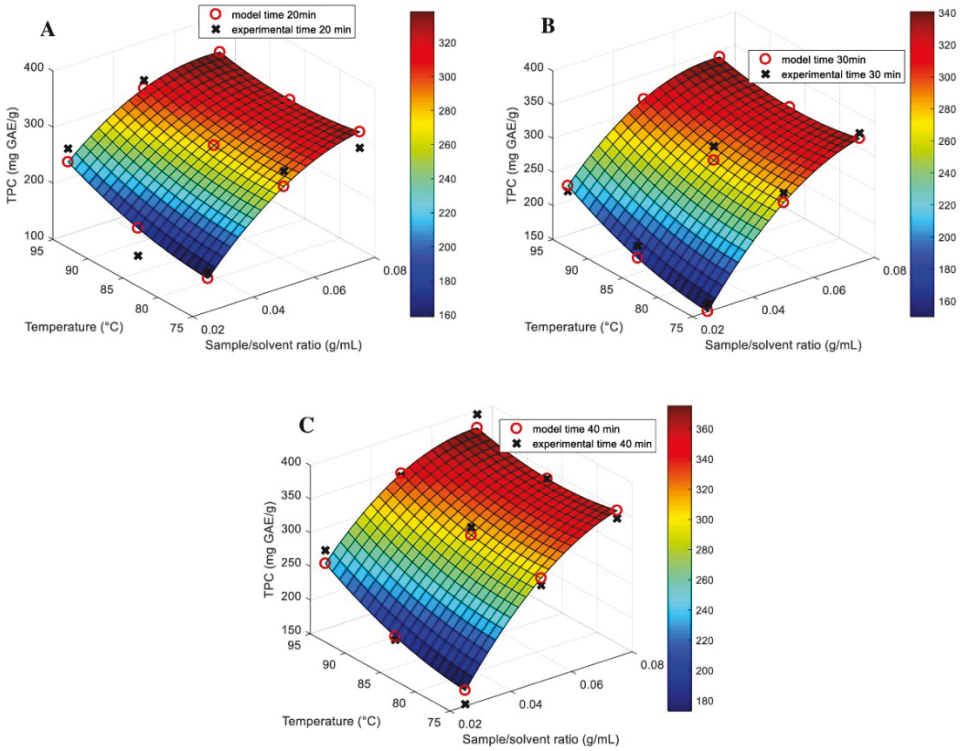

Figure 3. Interpolation and regression function of criterion K_1 (TPC, Total phenolic content) as a function of process parameters (decision variables) x_1 (Sample/solvent ratio ($g \cdot mL^{-1}$)) and x_3 (Temperature (˚C)) for: A – x_2=20 min (extraction time); B – x_2=30 min (extraction time); C – x_2=40 min (extraction time)

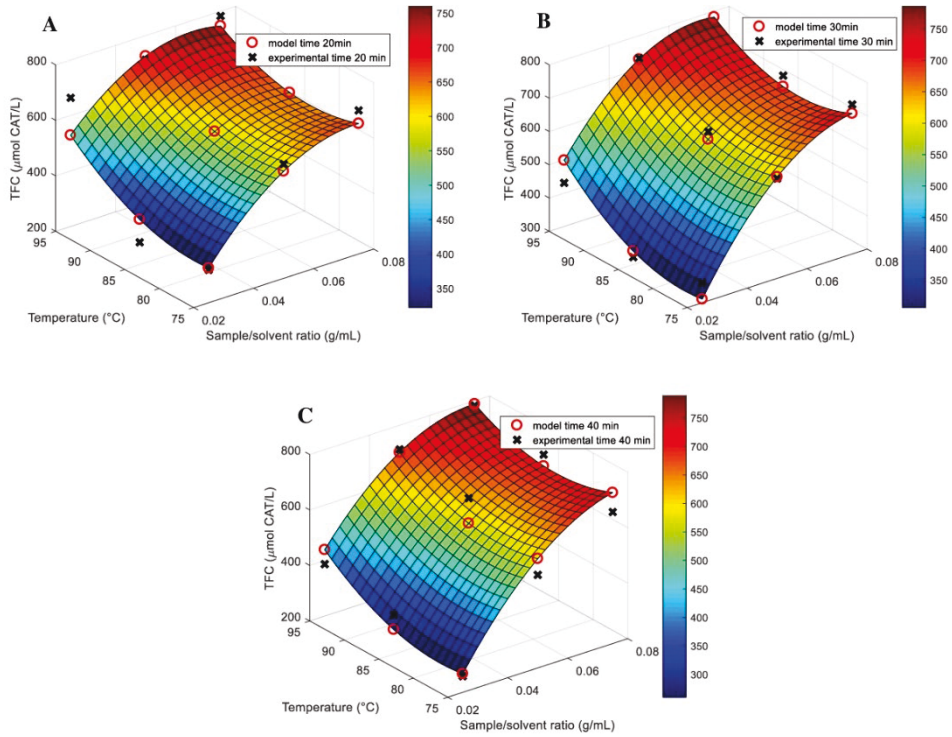

Figure 4. Interpolation and regression function of criterion K_2 (TFC, Total flavonoids content) as a function of process parameters (decision variables) x_1 (Sample/solvent ratio ($g \cdot mL^{-1}$)) and x_3 (Temperature (ºC) for: A – x_2=20 min (extraction time); B – x_2=30 min (extraction time); C – x_2=40 min (extraction time)

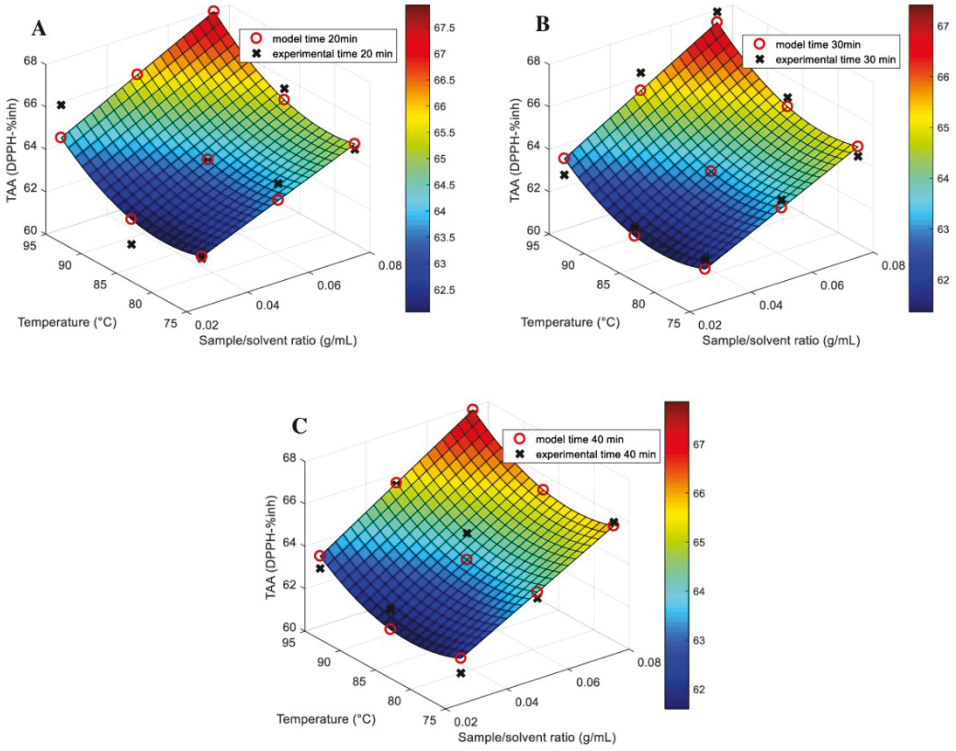

Figure 5. Interpolation and regression function of criterion K_3 (TAA, Total antioxidant activity) as a function of process parameters (decision variables) x_1 (Sample/solvent ratio ($g \cdot mL^{-1}$)) and x_3 (Temperature (ºC) for: A – x_2=20 min (extraction time); B – x_2=30 min (extraction time); C – x_2=40 min (extraction time)

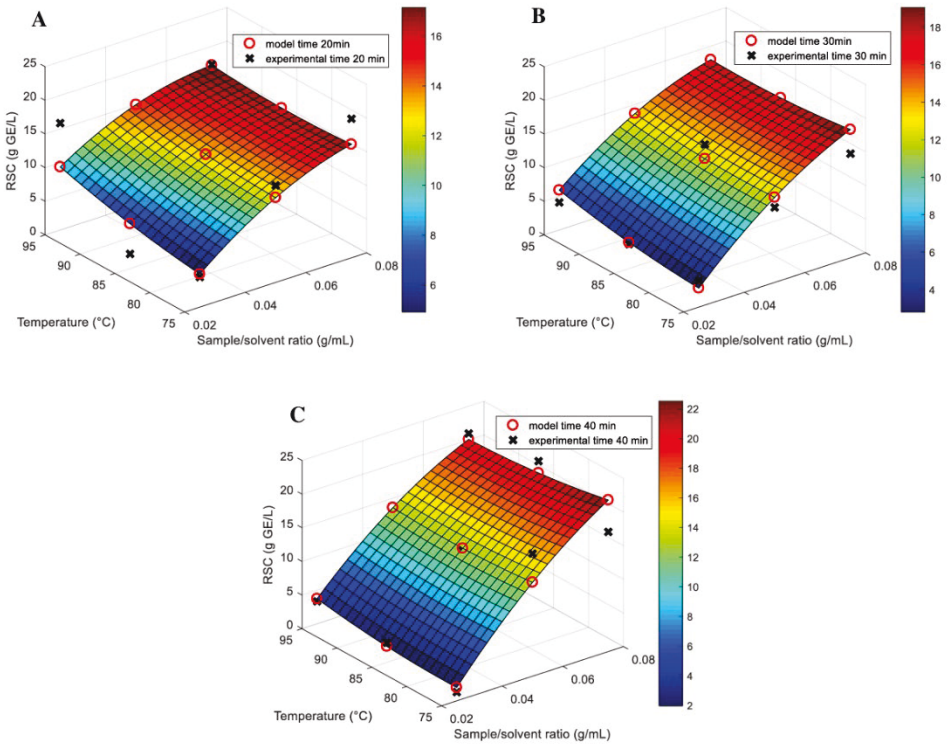

Figure 6. Interpolation and regression function of criterion K_3 (RSC, Reducing sugar content) as a function of process parameters (decision variables) x_1 (Sample/solvent ratio ($g \cdot mL^{-1}$)) and x_3 (Temperature (ºC) for: A – x_2=20 min (extraction time); B – x_2=30 min (extraction time); C – x_2=40 min (extraction time)

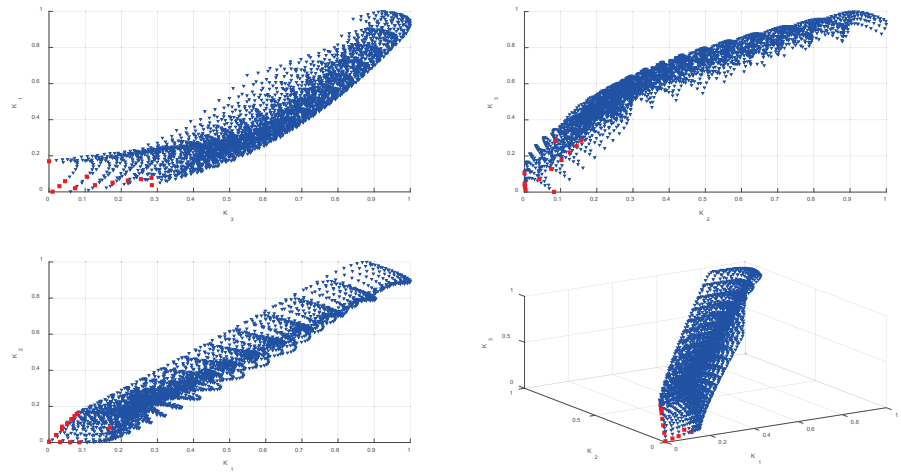

Figure 7. Sets of Pareto solutions for maximising regression equations for the relationship between criteria K_1 (TPC total phenolic content-maximised), K_2 (TFC total flavonoids content-maximised), K_3 (TAA total antioxidant activity-maximised). Red color indicates Pareto-optimal solutions (Pareto front), blue color indicates dominated solutions. For maximised criteria, 0 is the best case scenario

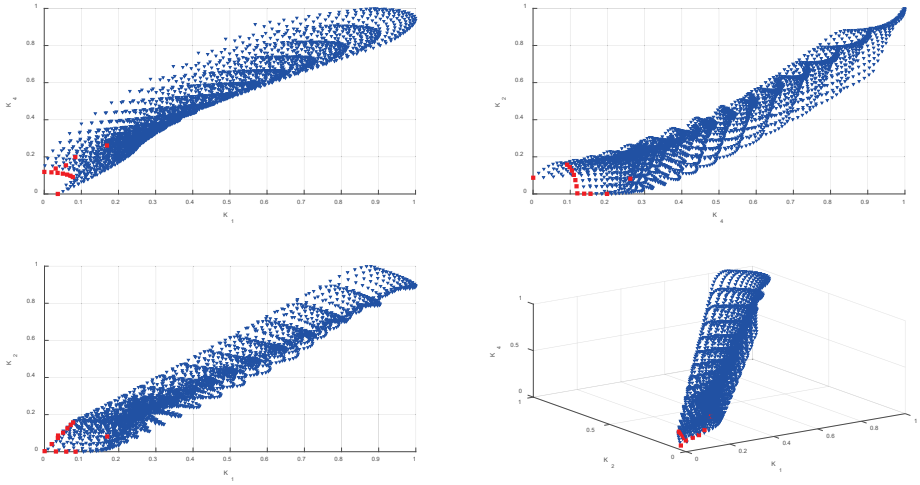

Figure 8. Pareto solution sets for maximising regression equations for the relationship between criteria K_1 (TPC total phenolic content - maximised), K_2 (TFC total flavonoids content - maximised), K_4 (RSC reducing sugar content). Red color indicates Pareto-optimal solutions, blue color indicates dominated solutions. For maximised criteria, 0 is the best case scenario

The set of all possible non-dominated i.e. Pareto-optimal solutions is shown in Figures 7-8 (selected sets of acceptable solutions from among all possible solutions for the object under consideration). The figures show local trends analysed in two or three dimensions, which was a transition from a 4-dimensional space. The maximised criteria were scaled so 0 was the best scenario. The red area reflects all acceptable Pareto-optimal solutions. Any value in the red area is considered optimal and can be selected as a process parameter. The blue area includes solutions that are dominated. These solutions are not optimal and will not provide the desired maximisation of extraction of biologically active compounds from *Levissticum officinale*.

The pareto-optimal solutions for the maximised criteria (K_1 – TPC total phenolic content, K_2 – TFC total flavonoids content, and K_3 – TAA total antioxidant activity) were close to zero. Maximisation of total phenolic content results in maximisation of total flavonoid content and maximisation of total antioxidant activity (Fig. 7). Furthermore, maximisation of the total flavonoids content leads to maximisation of total antioxidant activity (Fig. 7). From a practical point of view, this means that the use of low process temperatures and a lower biomass/solvent ratio will result in a lower content of TPC, TFC, and TAA in the final extract from *Levisticum officinale*. RSC reducing sugar content is another important aspect affecting the quality and activity of extracts. Figures 8 show a detailed analysis of the relationship between the criteria with the dominated solutions and the Pareto front. Based on the results, it was concluded that by controlling the parameters of the extraction process appropriately, it is possible to increase the concentration of individual biologically active compounds. The decision process will be facilitated by the determined explicit form of the set of dominated and non-dominated (Pareto-optimal) solutions for the water extracts in the decision criteria space, corresponding to K_1, K_2, K_3, and K_4.

Figure 7-8 shows the form of the set of dominated and non-dominated solutions for the extracts, demonstrating that there is a relatively small area of non-dominated solutions. To facilitate decision-making, the Pareto solution sets for the maximisation of the regression equations as a function, not of criteria, but of the variable decision variables x_1 (Sample/solvent ratio), x_2 (Time), and x_3 (Temperature) are shown on Figure 9 for the selection of the optimum water extraction parameter of *Levisticum officinale*.

Changing the space gives a clearer picture of the parameters affecting the maximisation of bioactive compounds in the extracts. It was shown that three options can be used for maximising criteria. Thus, increasing the process temperature, extending the extraction time, and increasing the plant biomass/solvent ratio will achieve extracts with optimised criterion values (maximising the level of bioactive compounds). The second route assumes that increasing the extraction time offers the possibility of lowering the temperature and decreasing the ratio of plant biomass to solvent, without loss to maximisation of criteria. The approach of possibly lowering the process temperature, increasing the extraction time and increasing the plant biomass/solvent ratio for Pareto-optimal solutions to maximising the criteria presented can also be applied.

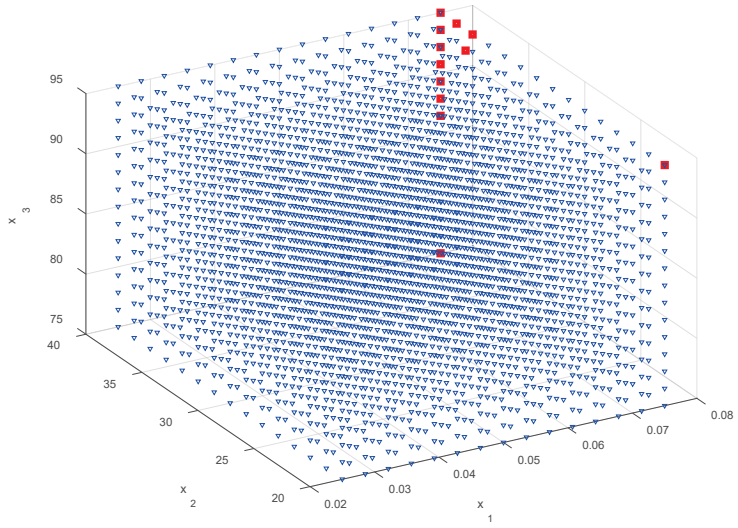

Figure 9. Pareto solution sets for maximising regression equations as a function of the decision variables x_1 (Sample/solvent ratio), x_2 (Time) and x_3 (Temperature). Red color indicates Pareto-optimal solutions, blue color indicates dominated solutions.

Thus, the determination of Pareto fronts showed that to maximise the extraction of bioactive compounds from the roots of *Levisticum officinale*, optimal extraction process parameters should be used, whose values were 0.0714 g·mL^{-1} as the biomass/water ratio and a time of 35.7142 min, at the highest temperature analysed (Table 2).

Table 2.
Set of decision variable values for Pareto front solutions

x_1 – Sample/solvent ratio (g·mL^{-1})	x_2 – Time (min)	x_3 – Temperature (ºC)
0.0714	35.7143	95.0000
0.0750	20.0000	95.0000
0.0750	37.1429	95.0000
0.0750	38.5714	95.0000
0.0750	40.0000	75.0000
0.0750	40.0000	86.4286
0.0750	40.0000	87.8571
0.0750	40.0000	89.2857
0.0750	40.0000	90.7143
0.0750	40.0000	92.1429
0.0750	40.0000	93.5714
0.0750	40.0000	95.0000

For the maximum analysed value of plant biomass and solvent ratio and the maximum process temperature, extraction can be carried out for 20 min or in the range 37.1429 - 38.5714 min. On the other hand, assuming that the extraction time reaches 40 min and the sample/solvent ratio 0.0750 $g \cdot mL^{-1}$, the process temperature is between 75ºC and 95ºC.

It should be emphasised that multi-objective optimisation finds many sets of possible solutions in the area of constraints imposed by the decision-maker. At this stage, there is the intention of the so-called post-optimisation analysis, i.e. the process of interpreting the results obtained and searching for a satisfactory solution. However, in both methods, in addition to the optimisation procedures, the knowledge and experience of those making the final decision are of inestimable importance. Figures 7-8 present a clear message about the high complexity of the research problem under consideration, which makes it directly difficult to choose a single best answer and to find a single best solution (sets were determined). Thus, of all the optimal solutions, the best solution can be selected in an infinite number of ways using a number of methods. One such method is, for example, VIKOR (San Cristóbal, 2011; Ramirez-Atencia et al., 2020). This method supports decision-making problems in which the criteria are, for example, incommensurable (have different units). In this method, the decision-maker seeks a compromise solution that is closest to the assumed ideal. In such cases, distances, are most often used as so-called cardinal measures. They can be repeznted by Euclidean, Chebyshev, or Manhattan distances (Szádoczki et al., 2023). Obtaining and analysing trade-off solutions is considered a relatively simple and effective method of selection and decision-making for decision-makers, as it provides a basis for an agreement based on mutual concessions (Szparaga et al., 2019). One assumption is that some Pareto points can be determined as 'better' than others. This leads to a so-called Pareto set reduction based on the development of an efficiency measure for each Pareto point. For the analysis of the process of aqueous extraction of bioactive compounds from the roots of *Levisticum officinale*, it was chosen to find compromise solutions using the method of multidimensional Euclidean metrics, i.e. achievable preferred solutions on the Pareto front with minimum distance from the Utopia point (d_U).

Figure 10 shows the Pareto-optimal solutions with a minimum distance from the Utopia point (compromise solutions).

It was shown that high values of the *Levisticum officinale* biomass-to-water ratio could be used in the extraction process to obtain satisfactory Pareto solutions (Fig. 10A), thus reducing the process time. On the other hand, the inverse relationship, resulting from the use of the minimum distance analysis from the Utopia point, indicated that increasing the time of the extraction procedure would ultimately allow a reduction in the amount of plant biomass consumed. This appears to be an extremely important finding from the Pareto-optimal solution set reduction method. This is because it translates into a smooth and intuitive ability to control the extraction process for satisfactory maximisation of the level of bioactive compounds with biostimulatory potential for crop plants.

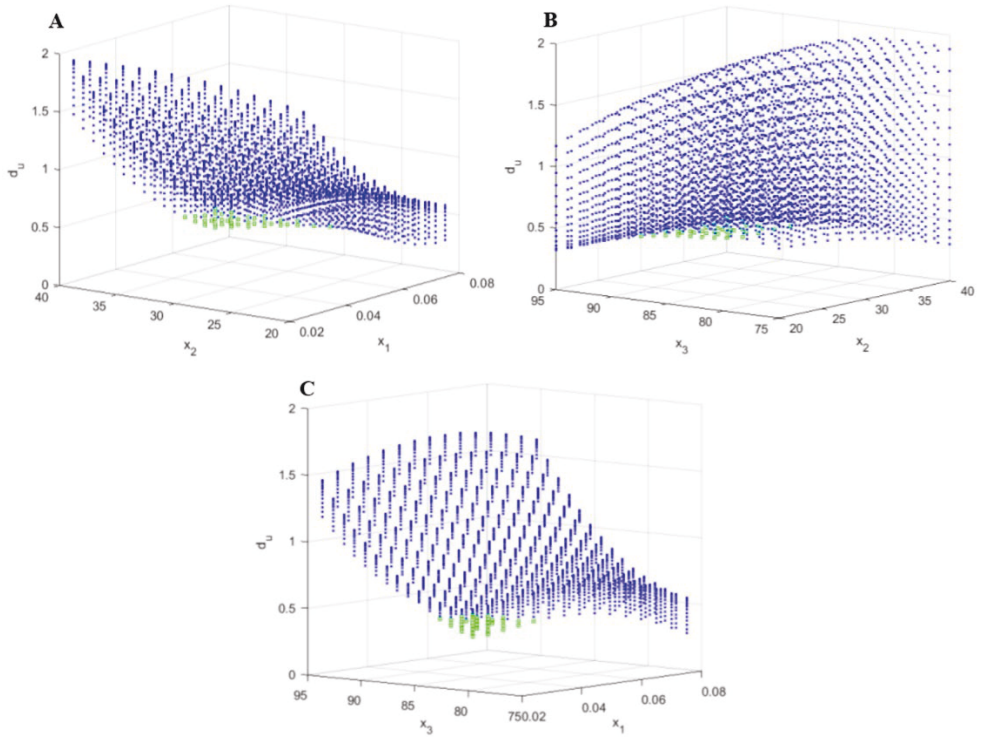

Figure 10. Sets of compromise solutions (d_U) as a function of the decision variables: A - x_1 (Sample/solvent ratio) and x_2 (Time); B – x_2 (Time) and x_3 (Temperature); C – x_1 (Sample/solvent ratio) and x_3 (Temperature)

Similar conclusions were reached in the subsequent analysis. It was found that to achieve satisfactory solutions from the set of Pareto-optimal solutions (Fig. 10B) for extraction, it is possible to use high values of temperature, which consequently leads to the possibility of reducing the process time. In addition, it was shown that a reduction in process time would be possible with higher temperatures. Similar possibilities for deciding on extraction process parameters have been demonstrated for the relationship between temperature and the ratio of root biomass to solvent. Indeed, it is possible to achieve satisfactory solutions by lowering the extraction temperature, but increasing the analytical biomass-to-water ratio (Fig. 10C). The above indications can be extremely valuable for the informed control of the process to maximise the bioactive compounds extracted.

The set of compromise solutions in 3D space (a system of three decision variables) is shown on Figure 11.

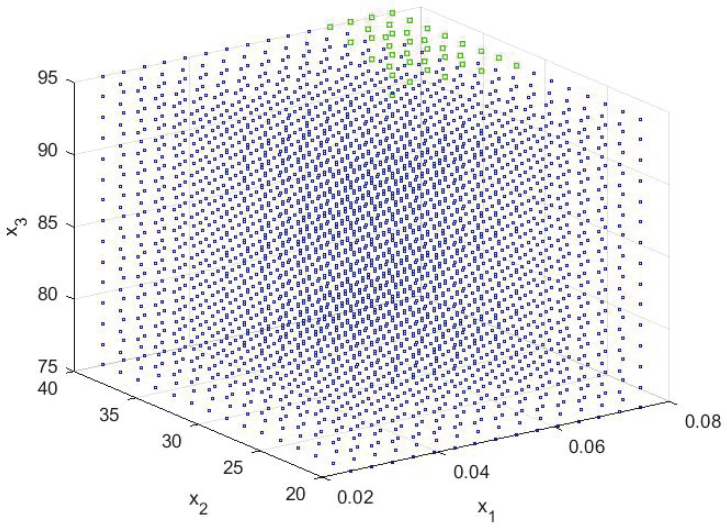

Figure 11. Illustration of compromise solutions based on distance from Utopia point as a function of decision variables x_1 (Sample/solvent ratio), x_2 (Time), and x_3 (Temperature). The green color indicates compromise solutions, the blue color indicates dominated solutions

It is shown that, through the role of the decision maker, a larger number of satisfactory trade-off solutions can be obtained, which will allow easier decision-making regarding the process of extracting active compounds from the roots of *Levisticum officinale*.

The compromise solutions in Table 3 are the number of solutions whose distance from the Utopia point was less than 0.29. The set of compromise solutions in the space of decision variables is shown in Table 3. It is possible to consider the obtained solutions as the best solution of all the Pareto solutions obtained in terms of satisfying all criteria.

Table 3.
Compromise solutions in the decision variables space

x_1 – Sample/solvent ratio ($g \cdot mL^{-1}$)	x_2 – Time (min)	x_3 – Temperature (ºC)
0.0643	40.0000	95.0000
0.0679	37.1429	95.0000
0.0679	38.5714	95.0000
0.0679	40.0000	93.5714
0.0679	40.0000	95.0000
0.0714	32.8571	95.0000
0.0714	34.2857	95.0000
0.0714	35.7143	93.5714
0.0714	37.1429	95.0000

x_1 – Sample/solvent ratio ($g \cdot mL^{-1}$)	x_2 – Time (min)	x_3 – Temperature (ºC)
0.0714	37.1429	93.5714
0.0714	38.5714	95.0000
0.0714	38.5714	92.1429
0.0714	38.5714	93.5714
0.0714	40.0000	95.0000
0.0714	40.0000	92.1429
0.0714	40.0000	93.5714
0.0714	30.0000	95.0000
0.0750	31.4286	95.0000
0.0750	32.8571	95.0000
0.0750	32.8571	93.5714
0.0750	34.2857	95.0000
0.0750	34.2857	93.5714
0.0750	35.7143	95.0000
0.0750	35.7143	92.1429
0.0750	35.7143	93.5714
0.0750	37.1429	95.0000
0.0750	37.1429	92.1429
0.0750	37.1429	93.5714
0.0750	38.5714	95.0000
0.0750	38.5714	90.7143
0.0750	38.5714	92.1429
0.0750	38.5714	93.5714
0.0750	40.0000	95.0000
0.0750	40.0000	89.2857
0.0750	40.0000	90.7143
0.0750	40.0000	92.0143
0.0750	40.0000	93.5714
0.0750	40.0000	95.0000

In the available literature, there is little information on the use of multi-objective optimisation in extraction processes Mostly researchers use the Response Surface Methodology (RSM). Vázquez et al. (2012), Jerez et al. (2006), and Saha et al. (2011) found that when RSM methods were used to maximise phenolic compound extraction and antioxidant potential, there were discrepancies in the significance of the quadratic model coefficients, which they attributed to the particular structure and composition of the plant matrices, which contain different phenolic compounds as well as other components that can affect their extraction. Viacava et al. (2015) emphasized that, as each biological system may show a different response to extraction conditions, hence it is extremely important to optimise the process parameters in each plant matrix, assuming that not only different experimental design techniques but also post-optimisation analysis will be used.

Among the Pareto-optimal and compromise solutions (assuming that the objective function determined the simultaneous maximisation of antioxidant potential and bioactive compound levels), an increased value of the decision variable x_3 (process temperature) prevailed. This is reflected in a study by Chethan and Malleshi (2007), who confirmed that elevated temperatures enhance the extraction process of bioactive compounds, which they linked to the fact of increased solubility, increased diffusion coefficients, and reduced surface tension. According to the researchers, the higher extraction efficiency of phenolic compounds may also be due to the weakening of bonds between phenols and carbohydrates. However, a study by Viacava et al. (2015), in which they analysed the critical parameters for extraction processes, showed that increasing the process temperature enhanced the extraction of antioxidant compounds, but that individual types of extraction, including the type of solvent used, should be analysed (Chethan and Malleshi, 2007).

Extending the discussion on optimization, it should be emphasized that other process parameters should also be considered in future studies. According to Plaza and Turner (2017), the influence of, among other things, the possible addition of certain organic or inorganic modifiers or surfactants, which can determine the efficiency of extraction of biologically active compounds from plant matrices, should also be evaluated. An aspect to be considered in the future is also the extraction ocean and its optimization in terms of sample fineness. Preliminary reports by Gbashi et al. (2020) indicate that a smaller particle size results in increased contact area between the sample and the extractant. Additionally, as indicated by Vázquez et al. (2020), more attention in extraction design, as well as its optimization, should be paid to determining the solvent to plant biomass ratio and developing such biomass fractions without the constant need to replace the extractant with fresh solvent.

According to Plaza and Turner (2017), it is noteworthy that often a higher solvent-to-sample ratio will result in the need to heat a larger volume of water. The researchers also point out that in such a case, the analyte will be less concentrated in the extract, so a concentration step may be necessary, which carries a higher risk of degradation of bioactive compounds.

Wani and Uppaluri (2022) suggested a direction for further research on the extraction process and its optimization. The authors pointed out that the moisture content of the plant sample itself may also be a parameter that can determine the efficiency of aqueous extraction. Indeed, the first studies showed that plant biomass, characterized by higher levels, leads to extracts more abundant in phenolic compounds, with respect to dried samples.

To summarise the research, it should be pointed that extraction optimisation is an extremely important tool for supporting process design in terms not only of the economic side, associated with controlling process parameters, but also in terms of producing satisfactory products for many applications (food, pharmaceutical, agricultural). Multi-objective optimisation and multi-criteria decision analysis providing to the identification of unacceptable (for the final quality of the product) extraction process parameters. This approach also reduces the need to conduct many costly and time-consuming experimental studies. In addition, the graphical visualisation of Pareto-optimal and compromise solutions are extremely important and helpful not only in the sense of deciding which solutions to choose but also enables relatively intuitive observation and identification of relationships between variables and different biological system responses and criteria (Ribeiro et al., 2008).

Conclusions

Aqueous extraction of plant biomass is a complex process influenced by many factors. In the research, extraction based on green procedures was analysed for maximising the extraction efficiency of total phenols, flavonoids, sugars, and antioxidant potential from the roots of *Levisticum officinale*, using water as an environmentally friendly solvent. Due to the current attention to the principles of green chemistry and in line with the European Green Deal, the application of optimisation methods tends into these research trends, due to the support of process design, taking into account the reduction of its immediate and long-term environmental impact. Multi-objective optimisation of aqueous extraction has been shown to be an extremely useful technique for determining the optimal process conditions to obtain *Levisticum officinale* root extracts with maximum levels of biologically active compounds. This approach also provides a wide range of information about the process, without the need for multiple experiments. Such a procedure is extremely important in terms of the potential use of plant extracts in many fields and industries. The results of the tests carried out showed that the procedures adopted for modelling the influence of individual process factors on the criteria analysed were correct, and the generated models reflected the process to satisfactory degree. Thus, they could be used for Multi-objective optimisation, in which the decision variables of the process were optimised for the maximisation of the individual criteria. The optimisation procedures showed that the high complexity of the research problem under consideration, which directly hinders the selection and the finding of a single best solution. Thus, sets of solutions were determined. The Pareto front analysis showed that for the maximum extraction efficiency of bioactive compounds from *Levisticum officinale*, the optimal extraction process parameters were 0.0714 $g \cdot mL^{-1}$ as biomass/water ratio and a time of 35.7142 min, with the highest analysed temperature. For the highest analysed value of plant biomass/solvent ratio (0.075 $g \cdot mL^{-1}$) and maximum process temperature (95ºC), extraction could be carried out for 20 min or in the range 37.1429 - 38.5714 min. On the other hand, assuming the extraction time reaches 40 min and a sample/solvent ratio of 0.075 $g \cdot mL^{-1}$, the optimum process temperature is between 75ºC and 95ºC. In conclusion, conventional extraction can be used as a safe method (not requiring the use of environmentally harmful solvents) to produce bioactive-rich extracts from *Levisticum officianale*. The optimised extracts can be used to develop new biostimulant formulations for agriculture functional foods or natural cosmetics.

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WIELOOBIEKTOWA OPTYMALIZACJA WARUNKÓW ZIELONEJ EKSTRAKCJI ZWIĄZKÓW BIOAKTYWNYCH Z *LEVISTICUM OFFICINALE* WDJ KOCH: OPTYMALNOŚĆ PARETO I ROZWIĄZANIA KOMPROMISOWE W ZARZĄDZANIU PROCESAMI

Streszczenie. Rośliny należące do rodziny Apiaceae (w tym *Levisticum officinale* WDJ Koch) są bogatym źródłem fitochemikaliów i metabolitów wtórnych o potencjalnym potencjale prozdrowotnym i agrochemicznym. Celem niniejszej pracy było dostarczenie ważnych wytycznych dotyczących kontrolowania konwencjonalnej ekstrakcji wodnej w celu uzyskania ekstraktów z korzenia *Levisticum officinale* o zmaksymalizowanych poziomach związków bioaktywnych. Dlatego też w niniejszym badaniu oceniono i zoptymalizowano potencjał przeciwutleniający wodnych ekstraktów z *Levisticum officinale* pod kątem analizy wpływu parametrów procesu ekstrakcji, tj. temperatury, czasu i stosunku biomasy roślinnej do rozpuszczalnika. Ostatecznym celem była optymalizacja całkowitej zawartości związków fenolowych, flawonoidów, cukrów i całkowitej zdolności przeciwutleniającej w celu zidentyfikowania warunków procesu niezbędnych do wytworzenia wysoce bioaktywnych ekstraktów, które mogłyby być stosowane w wielu gałęziach przemysłu. Ekstrakcję biomasy korzenia lubczyku przeprowadzono przy użyciu wody jako rozpuszczalnika ekstrakcyjnego. Aby przeprowadzić optymalizację ekstrakcji wodnej, zastosowano wielowymiarowe modele regresji i przeprowadzono analizę wielokryterialną przy użyciu nawigacji zestawu Pareto. Procedury optymalizacyjne wykazały dużą złożoność rozważanego problemu badawczego, co bezpośrednio utrudnia wybór jednego najlepszego rozwiązania. W związku z tym wyznaczono zbiory rozwiązań. Analiza frontu Pareto wykazała, że dla maksymalnej wydajności ekstrakcji związków bioaktywnych z *Levisticum officinale*, optymalnymi parametrami procesu ekstrakcji były 0,0714 $g \cdot ml^{-1}$ jako stosunek biomasy do wody oraz czas 35,7142 min, w najwyższej analizowanej temperaturze. Dla najwyższej analizowanej wartości stosunku biomasy roślinnej do rozpuszczalnika (0,075 $g \cdot ml^{-1}$) i maksymalnej temperatury procesu (95ºC), ekstrakcję można było prowadzić przez 20 min lub w zakresie 37,1429-38,5714 min. Z drugiej strony, jeśli czas ekstrakcji osiągnie 40 min, a stosunek próbki do rozpuszczalnika 0,075 $g \cdot ml^{-1}$, optymalna temperatura procesu wynosi od 75ºC do 95ºC.

Słowa kluczowe: ekstrakcja wodą, modelowanie, optymalizacja, optymalność Pareto, lubczyk