International Journal of Advanced Research in Science, Engineering and Technology

ISSN: 2350-0328

Vol. 12, Issue 7, July 2025

# Mathematical Optimization of the Extraction Process of Lignocellulosic Plant Raw Materials under Water Vapor Pressure

**Dilnavozkhon Ruziboeva, Nematjon Valiev**

PhD student, Department of Chemistry of the Kokand State University, 150700, Kokand, Fergana region, Republic of Uzbekistan

Associated Professor, PhD in chemical engineering, Department of Chemistry of the Kokand State University, 150700, Kokand, Fergana region, Republic of Uzbekistan

**ABSTRACT:** This article presents a comprehensive study on the results obtained through mathematical planning of experiments aimed at optimizing the extraction process of plant raw materials – specifically, the bark of white willow (*Salix alba*). The primary objective of this research was to determine the optimal conditions for obtaining a dry residue rich in extractive substances, which are of significant interest due to their potential pharmacological and industrial applications. To achieve this goal, the method of 3×3 Latin squares was employed as a robust statistical tool for the design and optimization of experiments. This method allowed for the systematic variation and control of key process parameters while minimizing experimental error and ensuring the reliability of the results. Through this approach, the study was able to identify and quantify the influence of various coefficients – such as temperature, pressure, and extraction duration – on the efficiency and yield of the extraction process. The experimental part of the research was conducted using a specialized autoclave system, which enabled precise control over extraction conditions. The extraction was performed in the presence of both water and steam, creating an environment conducive to the effective breakdown and release of bioactive compounds from the plant matrix. During the experiments, the steam pressure was carefully maintained within the range of 0.12 to 0.15 MPa, which was determined to be optimal for ensuring high extraction efficiency without compromising the structural integrity of the extracted compounds.

## I. INTRODUCTION

Extraction of plant raw materials is one of the key stages in obtaining biologically active compounds for the pharmaceutical, food, cosmetic and veterinary pharmaceutical industries. In recent years, special attention has been paid to the development of environmentally friendly extraction methods that minimize the use of toxic organic solvents and reduce the negative impact on the environment. In this area, the use of water and water vapor as an extractant is a promising solution that combines efficiency and environmental friendliness. The use of water and water vapor for extraction allows you to avoid the use of harmful solvents, which significantly increases the safety of the final product and reduces waste disposal costs. In addition, carrying out the extraction process in an autoclave provides an increase in pressure and temperature, which accelerates the diffusion of target compounds from plant material and helps to increase the yield of the extract. High pressure helps reduce the viscosity and surface tension of water, improving the penetration of the solvent into the cellular structures of plants.

Thus, this extraction method is environmentally friendly and technologically efficient, which makes it attractive for scaling in industrial production. This paper examines the features of using water and steam under autoclave conditions for the extraction of plant materials, and analyzes the advantages and prospects of this approach.

Modern technologies for the extraction of plant materials are increasingly accompanied by the use of mathematical modeling and numerical methods to optimize and predict the characteristics of the process. Mathematical methods allow a more accurate description of the extraction kinetics, the effect of process parameters (temperature, pressure, time) on the yield and quality of the extract, as well as the mechanism of mass transfer in complex multicomponent systems. In particular, modeling of diffusion processes under high pressure and temperature conditions created in an autoclave helps to understand the dynamics of water or steam penetration into plant material and the extraction of bioactive components. The use of mass transfer and heat exchange equations allows optimizing extraction modes, minimizing energy costs and processing time with maximum product yield. Moreover, the use of numerical methods and optimization algorithms makes it possible to conduct virtual experiments, which reduces the need for expensive and labor-intensive laboratory studies. This contributes to the accelerated implementation of environmentally friendly and energy-efficient extraction technologies at the industrial level.

Thus, mathematical modeling is an important tool for improving the efficiency and sustainability of water and steam extraction processes, providing deep understanding and control of process parameters.

Based on the above, the goal of this work is to study and optimize the extraction process of plant raw materials - white willow bark - *Salix alba* to obtain a dry residue of extractive substances using water and steam under autoclave conditions, with an emphasis on the environmental friendliness of the method and increased efficiency through the use of mathematical modeling of kinetics and mass transfer.

## II. LITERATURE SURVEY

The white willow plant – *Salix alba* is a representative of the genus of woody plants of the willow family – Salicaceae [1]. It is widely known for its medicinal properties and is used in traditional medicine of many cultures. The main raw material for obtaining bioactive compounds is willow bark, which is rich in various biologically active substances, including phenolic compounds, flavonoids, salicin and tannins [2]. These components have pronounced anti-inflammatory, analgesic and antimicrobial activity, which is confirmed by numerous pharmacological studies [3]. Particular attention in pharmacology is paid to tannins from willow bark. Tannins are polyphenolic compounds with antioxidant properties, the ability to bind proteins and modulate inflammatory processes. Their use in medical preparations is due to the pronounced ability to reduce irritation of the mucous membranes and have a protective effect on tissues [4,5].

Various extraction methods are used to extract bioactive components from willow bark, with organic solvents traditionally used. However, there is growing interest in more environmentally friendly technologies, including extraction using water and high-pressure steam, which allows preserving the biological activity of substances and reducing the toxicity of the product [6,7]. In recent years, considerable attention has been paid to the introduction of mathematical methods for modeling and optimizing the extraction processes of plant materials. For example, in [8], a kinetic model for the extraction of polyphenols from green tea leaves was developed, which made it possible to describe the dynamics of diffusion and evaluate the effect of temperature and time on the yield of the extract. Similarly, a study [9] demonstrated the effectiveness of numerical modeling for optimizing the extraction of antioxidants from oak bark using pressurized steam, which made it possible to significantly reduce the processing time while maintaining a high yield of active substances.

The use of mass transfer and heat exchange models was also applied in the work [10], where a complex mathematical model of plant raw material extraction was created, taking into account the influence of pressure, temperature and particle size of the raw material. Such a model made it possible to predict the concentration of target components at different stages of the process and adapt the extraction parameters for maximum efficiency.

Thus, the use of mathematical modeling and numerical methods is becoming an integral part of the development of new and improvement of existing technologies for the extraction of plant raw materials, providing a deeper understanding of mass transfer processes and allowing the creation of environmentally friendly, economical and highly efficient methods for obtaining valuable components.

## III. RESEARCH METHODOLOGY

Dry, crushed, prepared in accordance with the requirements, white willow bark - *Salix alba* were used as plant raw materials for the research. Samples were collected in March from tree branches cut off as a result of gardening work, growing along agricultural plantations. Samples of raw materials crushed to a size of 2-5 cm, 100 g each, were placed in a metal vessel made of stainless steel, filled with 500 ml of distilled water. The vessel with the sample was placed in a hermetic, thermostatic extractor equipped with a pressure gauge and a thermometer. The thermostat must be equipped with a working and emergency valves to protect against excessive water vapor pressure. Thus, the thermostat heats up to 120 ° C and the pressure can rise to 0.15 megapascals, at the same time the temperature of the plant material rises and the pressure is in the specified values.

The following factors were investigated:

$A$ – temperature, ºC, where $A_1 = 110$, $A_2 = 115$, $A_3 = 120$;

International Journal of Advanced Research in Science, Engineering and Technology

ISSN: 2350-0328

IJARSET IMPACT FACTOR 6.684

Vol. 12, Issue 7, July 2025

$B$ – pressure, MPa, where $B_1 = 0{,}13$, $B_2 = 0{,}14$, $B_3 = 0{,}15$;
$C$ – time at maximum, minutes, where $C_1 = 40$, $C_2 = 50$, $C_3 = 60$.

To conduct the experiment, extraction was carried out under different conditions, in 9 different variations. The experiments were planned according to the scheme given in Table 1.

**Table 1. Scheme of the experimental plan.**

| ***A*** | ***B*** | | |
|---|---|---|---|
| | $B_1$ | $B_2$ | $B_3$ |
| $A_1$ | $C_1$ | $C_3$ | $C_2$ |
| $A_2$ | $C_3$ | $C_2$ | $C_1$ |
| $A_3$ | $C_2$ | $C_1$ | $C_3$ |

## IV. EXPERIMENTAL RESULTS

**Table 2. Experimental results and some of their values**

| Experiments and meanings | $B_1$ | $B_2$ | $B_3$ | $_ATij$ sum | Average |
|---|---|---|---|---|---|
| $A_1$ | 9,9 | 12,6 | 12,0 | 34,5 | 11,5 |
| $A_2$ | 10,7 | 10,5 | 11,2 | 32,4 | 10,8 |
| $A_3$ | 11,8 | 10,4 | 10,5 | 32,7 | 10,9 |
| $_BTij$ sum | 32,4 | 33,5 | 33,7 | $T = 99{,}6$<br>$N = 9$<br>$f = 2$ | |
| Average | 10,8 | 11,167 | 11,233 | | |
| $C$ factor | $C_1$ | $C_2$ | $C_3$ | | |
| $_CTij$ sum | 31,5 | 34,3 | 33,8 | | |
| Average | 10,5 | 11,433 | 11,267 | | |

To establish the significance of the influence of factors, dispersion analysis of the experimental results was carried out. Initial data for dispersion analysis:

$$T = \sum_{i=1}^{n} Tij \quad \text{(Formula 1)}$$

$$T = 31{,}5 + 34{,}3 + 33{,}8 = 99{,}6$$

An analysis of variance of the squares of all observation results was carried out using formula 2:

$$S^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} Yij^2 \quad \text{(Formula 2)}$$

$$S^2 = 9{,}9^2 + 12{,}6^2 + 12^2 + 10{,}7^2 + 10{,}5^2 + 11{,}2^2 + 11{,}8^2 + 10{,}4^2 + 10{,}5^2 = 1108{,}6$$

Then the sum of squares for each factor was determined using formula 3:

$$S_1^2 = \frac{1}{n} \sum_{i=1}^{n} T_A ij \quad \text{(Formula 3)}$$

After a series of calculations, we received the results:

$$S_1^2 = \frac{1}{n} \sum_{i=1}^{n} T_A ij = 1102{,}57$$

ISSN: 2350-0328

International Journal of Advanced Research in Science, Engineering and Technology

Vol. 12, Issue 7, July 2025

$$S_2^{\ 2} = \frac{1}{n}\sum_{i=1}^{n} T_B ij = 1103{,}10$$

$$S_3^{\ 2} = \frac{1}{n}\sum_{i=1}^{n} T_C ij = 1103{,}73$$

The mean value of the sum of squares for the obtained results was calculated:

$$\frac{T^2}{N} = \frac{99{,}6^2}{9} = \frac{9920{,}16}{9} = 1102{,}24$$

The values of the sums of squares were calculated using formula 4:

$$SS \ = S^2 - \frac{T^2}{N} \text{(Formula 4)}$$

Calculations and using formula 4 allow us to identify the total value of the sum of squares:

$$SS_{tot.} = S^2 - \frac{T^2}{N} = 6{,}36$$

also, the average value of each group of factors separately:

$$SS_A = S_1^{\ 2} - \frac{T^2}{N} = 0{,}16$$

$$SS_B = S_2^{\ 2} - \frac{T^2}{N} = 0{,}43$$

$$SS_C = S_3^{\ 2} - \frac{T^2}{N} = 0{,}74$$

After all observations, the variance residual is:

$$SS_{rem.} = SS_{com.} - SS_A - SS_B - SS_C = 1{,}84\bar{3}$$

To identify the F-values of the factors, a series of calculations were carried out using the derivatives below.:

$$S_A = \frac{SS_A}{f} \qquad f = \text{n} - 1; \qquad S_A = \frac{0{,}16}{2}$$

$$S_B = \frac{SS_B}{f} \qquad f = \text{n} - 1; \qquad S_B = \frac{0{,}43}{2}$$

$$S_C = \frac{SS_C}{f} \qquad f = \text{n} - 1; \qquad S_C = \frac{0{,}74}{2}$$

$$S_{rem.} = \frac{SS_{rem.}}{f} \qquad f = (\text{n} - 1)\ (\text{n} - 2); \qquad S_{rem.} = \frac{1{,}84\bar{3}}{2}$$

International Journal of Advanced Research in Science, Engineering and Technology

ISSN: 2350-0328

Vol. 12, Issue 7, July 2025

Now, F – is the value of the factors after calculations:

$$F_A = \frac{S_A}{S_{rem.}} = 0{,}09$$

$$F_B = \frac{S_B}{S_{rem.}} = 0{,}23$$

$$F_C = \frac{S_C}{S_{rem.}} = 0{,}40$$

To determine the significance of each factor, the F value was compared with the Fisher table criterion. The coefficient is significant if its absolute value is greater than the Fisher criterion ($F_{tab.}$ = 4.3). The results are presented in Table 3.

**Table 3. Significance of coefficients**

| $F_{exp.}$ – Fisher criterion | | Icons | $F_{tab.}$ – Fisher criterion | Results |
|---|---|---|---|---|
| $F_A$ | 0,09 | < | 4,3 | The coefficient is insignificant |
| $F_B$ | 0,23 | < | 4,3 | The coefficient is insignificant |
| $F_C$ | 0,40 | < | 4,3 | The coefficient is insignificant |

As can be seen, all factors investigated in the process turned out to be insignificant.

Next, to increase the efficiency of the process, the conditions of the extraction process were changed. For this, the crushed plant material was moistened with a 0.5% aqueous solution of sulfuric acid, since this concentration of acid is not so high as to completely hydrolyze organic bioactive plant compounds, but is sufficient for partial hydrolysis of high-molecular compounds. Such a solution should affect the yield of extractive substances, and subsequently the significance of the coefficients of the influencing factors. The experimental plan remains the same (Table 1).

The results of experiments using a low-concentration acid solution are collected in a table (Table 4), and their total and average values are also revealed..

**Table 4. Experimental results and some of their values**

| Experiments and meanings | $B_1$ | $B_2$ | $B_3$ | $_ATij$ sum | Average |
|---|---|---|---|---|---|
| $A_1$ | 9,5 | 10,2 | 12,1 | 31,8 | 10,6 |
| $A_2$ | 9,7 | 10,8 | 11,2 | 31,7 | 10,567 |
| $A_3$ | 13,6 | 13,8 | 14,5 | 41,9 | 13,967 |
| $_BTij$ sum | 32,8 | 34,8 | 37,8 | $T$ = 105,4<br>$N$ = 9<br>$f$ = 2 | |
| Average | 10,933 | 11,6 | 12,6 | | |
| $C$ factor | $C_1$ | $C_2$ | $C_3$ | | |
| $_CTij$ sum | 34,5 | 36,5 | 34,4 | | |
| Average | 11,5 | 12,167 | 11,467 | | |

According to formula 1, the significance of the influence of factors was established and a dispersion analysis of the experimental results was performed. Initial data for dispersion analysis: $T$ = 32,8 + 34,8 + 37,8 = 105,4. An analysis of variance of the squares of all observation results was carried out using formula 2: $S^2 = 9{,}5^2 + 10{,}2^2 + 12{,}1^2 + 9{,}7^2 + 10{,}8^2 + 11{,}2^2 + 13{,}6^2 + 13{,}8^2 + 14{,}5^2 = 1262{,}52$.
Then the sum of squares for each factor was determined using formula 3, which led to the results: $S_1^2$ = 1238,57; $S_2^2$ = 1257,25; $S_3^2$ = 1235,29. The mean value of the sum of squares for the obtained results was calculated: 1234,351. The values of the sums of squares were calculated using formula 4: $SS_{tot.}$=28,12, and the average value of each group of factors separately: $SS_A$=2,11, $SS_B$=11,45, $SS_C$=0,47. The residual variance is equal to 0.12. The importance of factors $F$ after calculations: $F_A$ = 47,33, $F_B$ = 213,29; $F_C$ = 4,51.

Next, the determination of the significance of each factor was compared by F – value with the Fisher table criterion. The coefficient is significant if its absolute value is greater than the Fisher criterion (Ftab. = 4.3). The results are presented in Table 5.

**Table 5. Significance of coefficients**

| $F_{exp.}$ – Fisher criterion | | Icons | $F_{tab.}$ – Fisher criterion | Results |
|---|---|---|---|---|
| $F_A$ | 36,54 | > | 4,3 | The coefficient is significant |
| $F_B$ | 198,13 | > | 4,3 | The coefficient is significant |
| $F_C$ | 8,10 | > | 4,3 | The coefficient is significant |

As can be seen from Table 5, all coefficients became significant. The assumption that the acid solution with a low concentration should have increased the yield of extractive substances was fully justified. Higher concentrations of acid solutions would have subjected natural compounds to high or complete hydrolysis, which is an undesirable effect. Because with high or complete acid hydrolysis, the biological activity of plant substances sharply decreases or disappears altogether. Thus, the mathematical model is adequate and fully justified all expectations.

## V. CONCLUSION

The conducted studies confirmed that, following the modification of extraction conditions, all the coefficients in the developed mathematical model proved to be statistically significant. This statistical significance underscores the high degree of reliability and consistency of the experimental results obtained. It also suggests that the chosen experimental design and analytical approach were appropriate for capturing the complex relationships between the process variables and the extraction efficiency. Consequently, the mathematical model developed during this research demonstrated a high level of adequacy and robustness. It accurately reflected the behavior of the extraction system under the tested conditions and fully validated the initial scientific hypotheses regarding the influence of various parameters on the outcome of the process. This confirmation not only reinforces the credibility of the model but also highlights its practical utility. Therefore, the model can be considered a reliable and effective tool for optimizing the extraction conditions of biologically active substances from plant raw materials, particularly from the bark of white willow (*Salix alba*). Its applicability may extend beyond the scope of this specific study, offering valuable guidance for future research and industrial-scale extraction processes involving similar botanical sources.

## REFERENCES

[1] POWO (2025). “Plants of the World Online. Facilitated by the Royal Botanic Gardens, Kew. Published on the Internet; https://powo.science.kew.org/ Retrieved 24 June 2025.”
[2] N.Tawfeek et al. Phytochemistry, Pharmacology and Medicinal Uses of Plants of the Genus Salix: An Updated Review // Frontiers in Pharmacology, Volume 12 – 2021
[3] M.Zarger et al. Phytochemical investigation and growth inhibiting effects of *Salix alba* leaves against some pathogenic fungal isolates. *World J. Pharm. Pharmacol.* 2014, 3, 1320–1330.
[4] A.Zaiter et al. Antioxidant and antiacetylcholinesterase activities of different granulometric classes of *Salix alba* bark powders. *Powder Technol.* 2016301, 649–656. doi:10.1016/j.powtec.2016.07.014
[5] N.A.Zabihi et al. *Salix alba* attenuated oxidative stress in the heart and kidney of hypercholesterolemic rabbits. *Avicenna J. Phytomed.* 2018, 8, 63.
[6] E.Cherkasova et al. Ensuring the safety of grain raw materials used in the production of grain products. E3S Web of Conferences. 2023390.0, 2018. 10.1051/e3sconf/20233900, 2018.
[7] I.Buyanova et al. Ecological problems related to the safe processing of dairy raw materials and whey // E3S Web of Conferences 284, 02016, 2021
[8] Jun Xi et al. Kinetic modeling of pressure-assisted solvent extraction of polyphenols from green tea in comparison with the conventional extraction / Food Chemistry, Volume 166, 2015, Pages 287-291
[9] I.M.Aroso et al. Hydroalcoholic extracts from the bark of Quercus suber L. (Cork): optimization of extraction conditions, chemical composition and antioxidant potential. Wood Sci Technol 2017, 51, 855–872.
[10] Valiev N.V. Technologies for the production of substances of antiarrhythmin and dihydroatisine hydrochloride preparations: Author... diss. Dr. Philos. according to techn. Nauk // PhD in Tech. Sciences. Tashkent. – 2018.