

Mathematical Modeling of Bioactivation Process for Wood Raw Materials

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Abstract

By the method of mathematical planning of the experiment, the influence of bioactivating the raw material of wood particles with a silt mixture of activated sludge, as well as humidity, lignin content in the press composition and the pressing temperature was investigated. Linear regression equations are obtained which allow predicting the effect of the above factors on the properties of wood plastics without using resin. Optimal values of bioactivation, conditions and factors for obtaining wood plastics without resins with high performance properties by hot pressing were determined.

Introduction

In the woodworking industry, a large amount of waste is generated during the processing of wood (represented as sawdust, shavings, grinding dust, etc.) and reach 35% [1]. There are several uses of wood waste:

- production of wood composite materials with the use of thermosetting organic and mineral binders [2]: particleboard, wood fiber boards (fiberboard); Composite wood-polymer materials (press powders, wood preservative masses, wood-mineral composite materials (arbolite, fibrolite, cement-chipboards, gypsum-fibrous boards, gypsum-chipboards).

- production of wood-polymer composites, in which thermoplastic polymers (polyethylene, polypropylene, polystyrene, polyethylene terephthalate, polymethylmethacrylate, etc.) are used as a matrix, and woodworking waste is used as a filler [3].

A method for obtaining wood plastics without using synthetic resins (WP-WR) has been developed. There are several technologies known:

- a one-stage method for obtaining piezothermoplastics, developed at the Belarusian Technological Institute under the guidance of A.N. Minin [4];

- a two-stage method for producing plastics from hydrolyzed sawdust, developed at the Leningrad Forestry Academy under the direction of N.Ya. Solechnik [5];

- A method for obtaining ligno-carbohydrate plastics, developed in the ULTI under the leadership of VN. Petri [6];

- technology of the steam explosion, developed at the Institute of Wood Chemistry of the Latvian Academy of Sciences under the leadership of Ya.A. Gravitis [7].

The production of these materials is due to the presence of lignin in the wood filler. Activation of lignin in the preparation of WP-WR is possible in the presence of modifiers, both low-molecular (ammonia, carbamide, acids, etc.) and high-molecular (lignin, lignosulfonate, etc.) chemical substances [4 - 5].

The use of chemical reagents leads either to the delignification process [8], or to the destruction of lignin to the formation of organic substances [9], which does not allow to fully predict the properties of the resulting materials.

We proposed a one-stage method for obtaining WP-WR in closed molds. At the same time, the hypothesis of partial chemical activation of lignin is used.

To eliminate the low values of the visco-plastic properties of the press raw material, it can be solved with the help of preliminary biological transformation and partial destruction of crushed wood, i.e. its bioactivation [10]. For this, the use of:

- a) active sludge in the form of a silt mixture, which is an available source of microorganisms destructive to wood;
- b) preactivated lignin (by cavitation method).

At the same time, economic and ecological problems are solved: waste utilization (excess activated sludge, hydrolytic lignin, wood waste) and cheaper production of products from WP-WR with satisfactory physical and mechanical properties.

Earlier we established [11-13] that the following factors influence the process of formation of WP-WR with high physical and mechanical properties: pressure, temperature of hot pressing, humidity, granulometric composition and recipes of press raw materials.

Experimental part

In order to obtain mathematical models that establish the relationship between physical and mechanical properties of WP-WR on the basis of bioactivated press raw materials obtained by the hot method in closed compression molds. From the studied factors, an experiment planning matrix was compiled based on the regression five-factor mathematical planning of a fractional factorial experiment of the 2^{5-1} type [14].

Preliminary studies [11-13] allowed to determine the influence of the following factors: Z_1 - content of lignin,%, Z_2 - pressing temperature, ° C, Z_3 - sludge consumption,%, Z_4 - duration of soaking (activation) with silt mixture, day; Z_5 - humidity of the initial press raw materials, %.

The output parameters are: bending strength (P, MPa), hardness (T, MPa), modulus of elasticity under compression (E_c , MPa), water absorption (B), thickness swelling (L,%), toughness (A, kJ / m²).

According to the planning matrix (see Table 1), by the method of flat hot pressing in a closed mold, samples of disks in three parallels with a diameter of 90 mm and a thickness of 2 mm were obtained.

Physicomechanical parameters were determined for the samples obtained.

Table 1: Planning matrix and physical and mechanical properties of WP-WR (two-level five-factor fractional mathematical plan of Box-Wilson)

№	Z_1	Z_2	Z_3	Z_4	Z_5	X_1	X_2	X_3	X_4	X_5	Y(P)	Y(T)	Y(E_c)	Y(B)	Y(L)	Y(E_H)	Y(A)
1	4	190	10	30	16	-1	+1	-1	-1	+1	54,01	52,62	642,18	35,13	10,97	1087,42	0,36
	4	190	10	30	8	-1	+1	-1	-1	-1	49,52	37,22	426,35	35,68	15,45	1677,59	0,46
	4	170	10	30	8	-1	-1	-1	-1	-1	40,11	40,26	469,50	44,05	20,91	1711,72	0,72
	4	170	10	30	16	-1	-1	-1	-1	+1	55,30	35,01	395,26	48,70	16,51	1497,07	0,40
2	4	190	20	50	16	-1	+1	+1	+1	+1	68,70	47,08	565,94	32,76	11,15	2129,97	0,62
	4	190	20	50	8	-1	+1	+1	+1	-1	66,05	56,60	694,46	55,54	31,87	1814,72	0,77
	4	170	20	50	8	-1	-1	+1	+1	-1	66,39	91,97	1151,55	69,37	41,24	2044,55	0,89
	4	170	20	50	16	-1	-1	+1	+1	+1	46,00	99,56	1177,03	52,06	24,45	1340,23	0,71
3	20	190	10	30	16	+1	+1	-1	-1	+1	54,30	44,97	536,24	40,14	21,84	1353,00	0,36
	20	190	10	30	8	+1	+1	-1	-1	-1	52,31	71,41	903,33	40,66	32,61	2334,30	0,45
	20	170	10	30	8	+1	-1	-1	-1	-1	57,93	103,27	1084,32	78,95	67,81	1436,07	0,55
	20	170	10	30	16	+1	-1	-1	-1	+1	59,83	38,30	441,69	54,65	35,15	1450,03	0,39
4	20	190	20	50	16	+1	+1	+1	+1	+1	61,46	40,21	469,22	34,69	18,95	1763,74	0,38
	20	190	20	50	8	+1	+1	+1	+1	-1	55,40	48,54	586,83	30,48	26,83	1605,76	0,45
	20	170	20	50	8	+1	-1	+1	+1	-1	54,85	271,07	1794,35	35,45	29,25	2422,05	0,47
	20	170	20	50	16	+1	-1	+1	+1	+1	51,29	40,84	477,73	42,87	29,04	1231,99	0,37
5	12	180	15	40	12	0	0	0	0	0	52,05	47,14	567,16	38,29	22,97	1977,17	0,53
	12	180	15	40	12	0	0	0	0	0	51,66	51,10	622,75	42,67	27,21	2574,28	0,51

The results of the experiments and their analysis

All the experimental data were processed using the MicrosoftExcel application package [15]. The regression equations for significant optimization parameters, with an estimate of their reliability, are presented in Table. 2.

As can be seen from Table. 2 high reliability values for the optimization parameters (T, E_c , B, P, L, A) provide the basis for the application of a system of linear equations for describing the studied processes of the influence of variable factors on optimization parameters [14].

Based on the adequate regression equations, graphical dependency surfaces were constructed (other factors were fixed at the middle level), shown in Fig. 12.

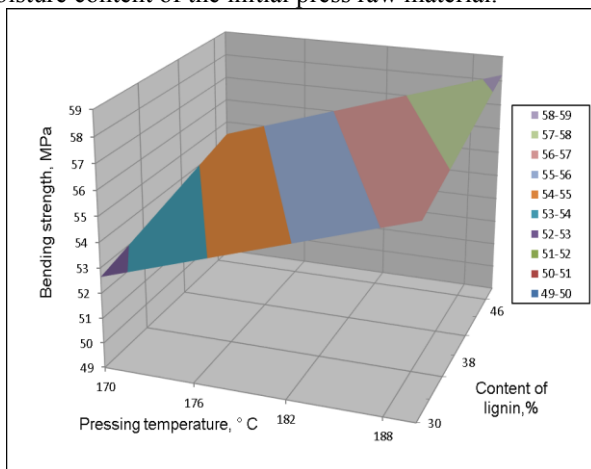
Table 2: Regression equations for significant optimization parameters with an estimate of their reliability

№	Optimization parameter	Equations of regressions with an estimate of their reliability
1	Y (P) - bending strength, MPa	$y(P) = -1,16 + 0,09 * Z_1 + 0,19 * Z_2 + 0,55 * Z_3 + 0,15 * Z_4 + 0,73 * Z_5$ $1-\alpha=0,95$
2	Y (T) - hardness, MPa	$y(T) = -479,68 + 9,76 * Z_1 + 2,49 * Z_2 + 6,7 * Z_3 + 3,3 * Z_4 + 1,38 * Z_5 - 0,05 * Z_1 * Z_2 - 0,009 * Z_2 * Z_3 - 0,23 * Z_3 * Z_4 - 0,05 * Z_4 * Z_5 + 0,03 * Z_5 * Z_1 - 0,03 * Z_1 * Z_3 + 0,01 * Z_1 * Z_4 - 0,06 * Z_3 * Z_5$ $1-\alpha=0,96$
3	Y (Ec) - modulus of elasticity under compression, MPa	$y(E) = -8312,36 + 136,7 * Z_1 + 45,02 * Z_2 + 255,89 * Z_3 + 65,84 * Z_4 - 26,87 * Z_5 - 0,8 * Z_1 * Z_2 - 1,07 * Z_2 * Z_3 - 4,20 * Z_3 * Z_4 - 0,51 * Z_4 * Z_5 + 1,2 * Z_5 * Z_1 - 0,08 * Z_1 * Z_3 - 0,11 * Z_1 * Z_4 + 0,62 * Z_3 * Z_5$ $1-\alpha=0,96$
4	Y (B) - water absorption,%	$y(B) = 166,67 + 0,11 * Z_1 - 0,74 * Z_2 - 0,21 * Z_3 - 0,22 * Z_4 + 0,97 * Z_5$ $1-\alpha=0,96$
5	Y (L) - swelling in thickness,%	$y(L) = -157,25 + 8,12 * Z_1 + 0,89 * Z_2 - 2,18 * Z_3 + 2,63 * Z_4 - 2,44 * Z_5 - 0,05 * Z_1 * Z_2 + 0,03 * Z_2 * Z_3 - 0,14 * Z_3 * Z_4 + 0,002 * Z_4 * Z_5 + 0,09 * Z_5 * Z_1 - 0,03 * Z_1 * Z_3 + 0,005 * Z_1 * Z_4 - 0,005 * Z_3 * Z_5$ $1-\alpha=0,98$
6	Y (A) - impact strength, kJ / m ²	$y(A) = -3,72 + 0,14 * Z_1 + 0,02 * Z_2 - 0,01 * Z_3 + 0,02 * Z_4 - 0,02 * Z_5 - 0,0007 * Z_1 * Z_2 + 0,0003 * Z_2 * Z_3 - 0,0018 * Z_3 * Z_4 + 0,0003 * Z_4 * Z_5 - 0,00006 * Z_5 * Z_1 - 0,0003 * Z_1 * Z_3 - 0,0001 * Z_1 * Z_4 + 0,001 * Z_3 * Z_5$ $1-\alpha=0,98$

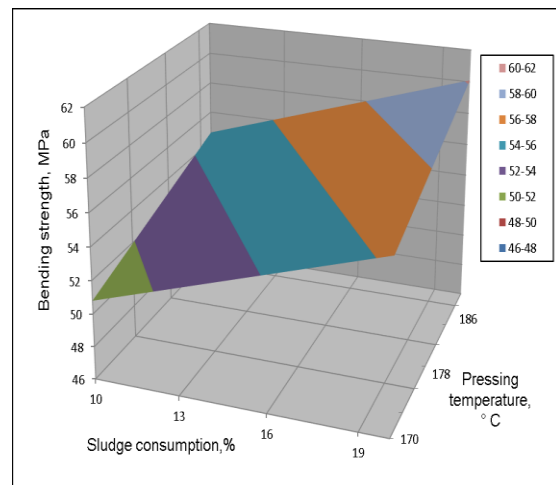
It is established that the strength at bending of the biactivated WP-WR significantly decreases with decreasing moisture of the press raw materials (see Fig. 1). This indicates the participation of water in the reactions of thermo hydrolytic degradation of the lignin-carbohydrate complex.

Increasing the duration of activating the press raw material with activated sludge (silt mixture) increases the bending strength of the WP-WR, since microorganisms (Actinomyces, Atcaligenes, Bacillus, Cellulomonas, Desulfotomaculum, Flavobacterium, Mycobacterium, Nocardia, Pseudomonas, Sarcina, etc.) containing in the silt mixture contribute to the partial destruction of lignin to the formation of functional groups. Pressing temperature WP-WR slightly affects the strength index of plastic.

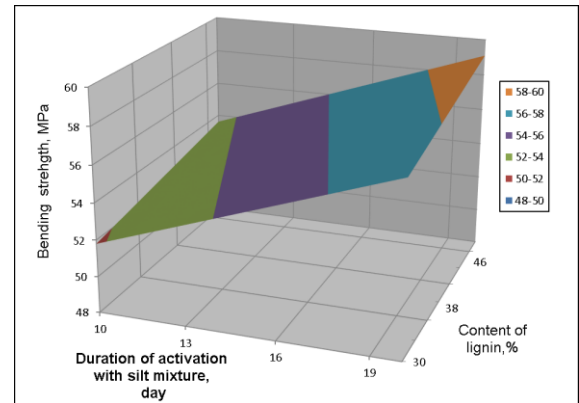
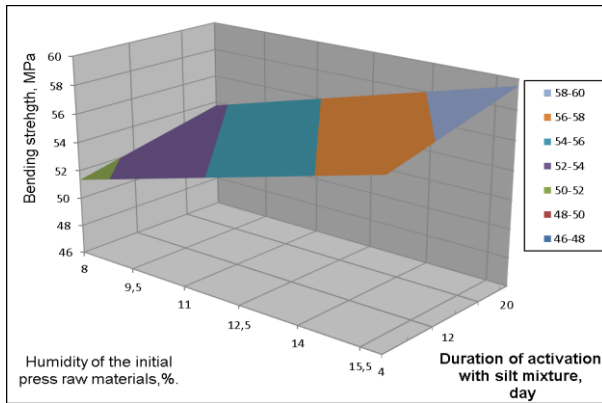
At the same time, water absorption increases with increasing raw material moisture and pressing temperature (see Figure 2), and high values of the hardness of the samples are achieved at the maximum temperature and minimum moisture content of the initial press raw material.



a)



b)

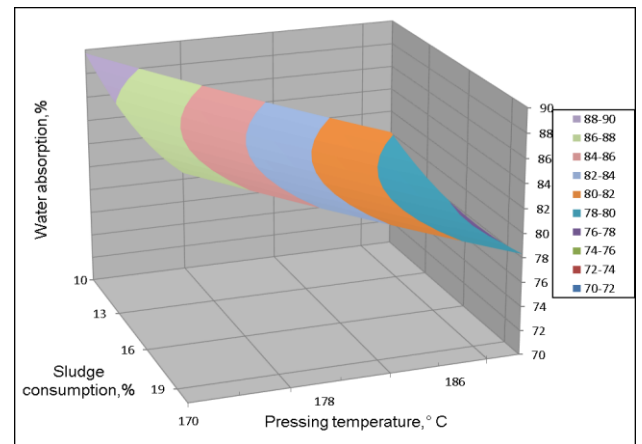
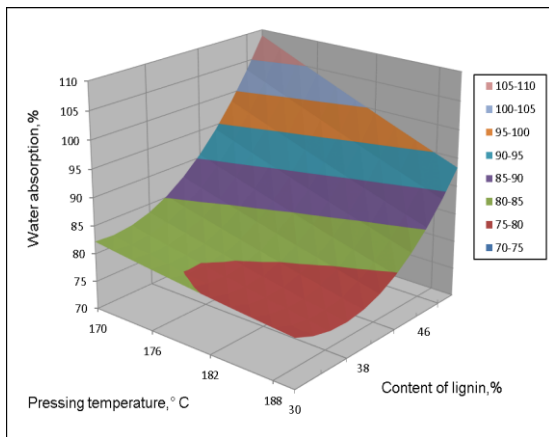


c)

d)

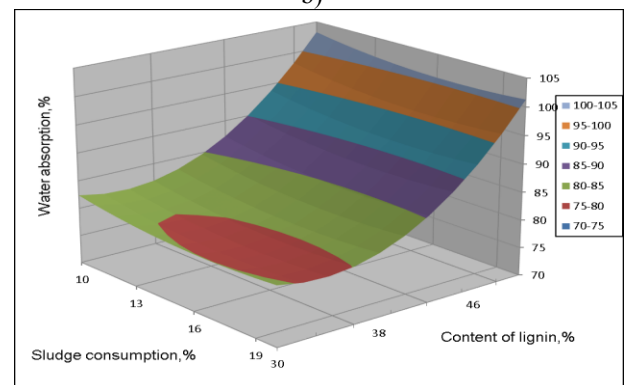
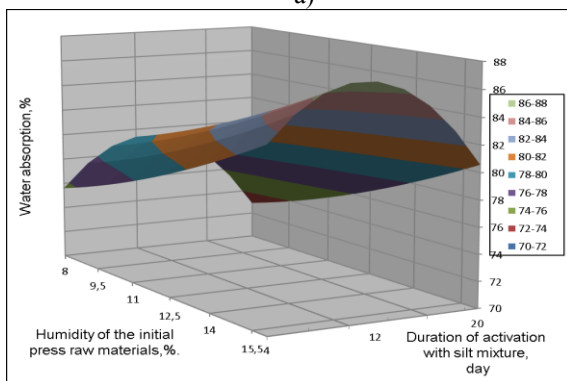
Figure 1: Dependence of the flexural strength of WP-WR from:

a) the influence of the pressing temperature and the content of cavitation lignin on the density; b) the influence of the flow of the silt mixture and the pressing temperature on the density; c) the influence of the moisture content of the press composition and the duration of bioactivation on the flexural strength; d) the effect of the duration of bioactivation and lignin content on the bending strength of WP-WR



a)

b)



c)

d)

Figure 2: Dependence of the water absorption of WP-WR on the effect:

a) the pressing temperature and the content of cavitation lignin; b) the flow rate of the sludge mixture and the temperature of pressing; c) humidity of the press composition and duration of bioactivation; d) humidity of the press composition and duration of bioactivation

The analysis of regression dependencies shows that the activation time of the press raw material with activated sludge (silt mixture) increases the compressive modulus, while the moisture content of the press raw material exerts more influence on this index than the pressing temperature.

Thus, it is established that the effect of the factors under study is differently directed to the physical and mechanical properties of WP-WR, and this requires an optimization approach. Therefore, using the method of linear programming, rational values of factors were determined.

The bending strength ($y(P)$) was used as the target function, while restrictions on other physical and mechanical properties of DP-BS (T, E_c, B, L, A) were established. The search for rational values was carried out in the range of the studied factors. Then the mathematical notation of finding rational values of factors has the form:

Target function: $y(P) = -1,16 + 0,09*Z_1 + 0,19*Z_2 + 0,55*Z_3 + 0,15*Z_4 + 0,73*Z_5 \rightarrow \max$

Restrictions: $y(T) \geq 60 \text{ МПа}$; $y(E) \geq 600 \text{ МПа}^2$; $y(B) \leq 40\%$; $y(L) \leq 30\%$; $y(A) \leq 0,35 \text{ кДж/м}^2$;

$4 \leq Z_1 \leq 20$; $170 \leq Z_2 \leq 190$; $10 \leq Z_3 \leq 20$; $30 \leq Z_4 \leq 50$; $8 \leq Z_5 \leq 16$.

Using the Microsoft Excel solution, the Solution Search application, a rational mode of obtaining WP-WR using bio-active activated wood raw material with active sludge (Table 3).

Table 3: Rational values of factors of obtaining WP-WR

№	Parameters	Values
1	Z_1 – Lignin content, %	30
2	Z_2 – Pressing temperature, °C	190
3	Z_3 – Sludge consumption, %	16
4	Z_4 – Activation duration, cyr	20
5	Z_5 – Moisture of press raw materials, %	16

Table 4 shows the calculated physico-mechanical properties of WP-WR at rational values of the factors.

Table 4: Calculated and experimental values of physical and mechanical properties of WP-WR

№	Parameter name	Calculated Values	Experimental values
1	Bending strength, MPa	61,0	59,1
2	Hardness, MPa	64,0	59,3
3	Modulus of elasticity under compression, MPa	638	486
4	Water absorption, %	37	31
5	Swelling in thickness, %	27	25
6	Impact strength, kJ / m ²	0,66	0,71

With the found rational values of the factors, samples of WP-WR were made and their physico-mechanical properties were determined (see Table 4).

Conclusion

Thus, bioactivation of wood raw materials with activated sludge leads to the appearance of functional groups in the structure of lignin, which then participate in the formation of WP-WR.

The obtained mathematical models establish the relationship between the physical and mechanical properties of the WP-WR and the factors studied (lignin content, sludge consumption, activation time, moisture of the press raw materials, pressing temperature), which is confirmed by the results of Table 4, that is, there is a good correlation between the calculated values with experimental values of plastic properties.

Bibliographic list

- [1]. State report "On the state and on the protection of the environment of the Russian Federation in 2016". - M.: Ministry of Natural Resources of Russia; NIA-Nature. - 2017. - 760 pp.
- [2]. Shcherbakov A.S. Technology of composite wood materials [text]: Textbook for high schools / A.S.Scherbakov, I.A.Gamova, A.V. Melnikova. - M.: Ecology, 1992. - 192 with. - ISBN 5-7120-0333-3.
- [3]. Klesov A. A. Wood-polymer composites. SPb.: Scientific foundations and technologies, 2010. - 736 p.
- [4]. Minin A.N. Technology piezotermoplastikov / AN Minin. - Moscow: Forest Industry, 1965. - 296 p.
- [5]. Plate materials and products made of wood and other dehydrated residues without adding binders / VN Petri [and others]. - Moscow: Forest Industry, 1976. - 360 p.
- [6]. Solechik N.Ya., Natkina L.N., Koromylova TS, Likhacheva L.I. On the receipt of wood plastic without a binder // Woodworking industry. 1963. № 3. P. 15-17

- [7]. Gravitis Ya.A. Theoretical and Applied Aspects of Explosive Autohydrolysis of Plant Biomass: (Review) // Timber Chemistry. 1987. № 5. P. 3-21.
- [8]. Popova, N.R. Catalytic oxidation of lignin substances using polyoxometallates as catalysts (review article) / N.R. Popova, K.G. Bogolitsyn, T.V. Povarnitsyna // Chemistry of plant raw materials. - 2008. - No. 4.- P. 5-14 - ISSN 1029-5143
- [9]. Kononov, G.N. Chemistry of wood and its main components: A teaching aid for students of specialties 2602.00, 2603.00 / G.N. Kononov. - Moscow: MGUL, 1999. - 247 p.
- [10]. Bolobova A.V. New technology for obtaining environmentally friendly building materials on the basis of enzymatic biodegradation of wood waste // Applied Biochemistry and Microbiology. 1999. Vol. 35. S. 590-595.
- [11]. Bioactivation of wood raw material with activated sludge to produce wood plastic without using resins / D.O. Gradinaru, A.V. Savinovskikh, A.V. Artemov, V.G. Buryndin, V. E. Artyomov // The forests of Russia and the economy in them. - 2013. - No. 44-1. - P. 126-129.
- [12]. Investigation of the physico-mechanical properties of wood-composite materials without using resins obtained on the basis of activated press raw materials / AV Savinovskikh, ZF Khusnutdinova, AV Artemov, OV Stoyanov, VG Buryndin // Bulletin of the Kazan Technological University. - 2014. - T. 17, No. 17. - P. 130-133
- [13]. Savinovskikh, A.V. The influence of modifiers on the physical and mechanical properties of wood plastics without using resins [Text] / A.V. Savinovskikh, A.V. Artemov, V.G. Buryndin // Bulletin of the Moskovsky State University Forest University - Lesnoy Vestnik. - 2016. - Vol. 20, No. 3. - P. 55-59
- [14]. Akhnazarova, S.L. Methods for optimizing the experiment in chemical technology / S.L. Akhnazarova, V.V. Kafarov. - M.: Higher education. Sc., 1985 - 327 p.
- [15]. Kuritsky B.Ya. Search for optimal solutions using Excel 7.0 / B.Ya. Kuritsky. S-Pb.: VNV - St. Petersburg, 1997.-384p.