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Kinetic Parameters of Smoke Aerosols during Combustion of Modified Wood

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Abstract. The most dangerous factors of fire are formation of smoke and thermal decomposition of toxic products. In case of fire, smoke spreads to evacuation routes. In this case, a person may be disoriented and feel panic. Smoke is an aerosol produced by the thermal decomposition of materials. The study object is the wood, which is widely used in construction. Up to date, the influence of wood species and wood surface layer modifiers on the smoke-forming ability has been studied. The effect of wood surface layer modifiers on the properties of aerosols remains insufficiently studied. The objective is to evaluate the effect of the wood surface layer modifiers on the formation and stability of smoke aerosols. In the course of work, the ultimate analysis method was used to assess the modifying effect of selected phosphoric acid esters. It is known that these compounds constitute effective flame retardants and are able to provide the biological stability of the wood. Granulometric analysis was additionally performed to evaluate the aerosol's properties. To evaluate the energy characteristics of the modified wood surface, the "neutral drop" method was used. As a result of the studies, a percentage phosphorous content was obtained in the surface layer of the wood before and after thermal decomposition. This data made it possible to conclude that the thermal effect of diethyl phosphite is very effective and stable when it is used as a modifier. Based on the granulometric analysis, the size distribution of solid aerosol particles was obtained. When using the selected modifiers, the maximum particle size of the aerosol is reduced, which in turn reduces the optical density of the smoke. Phosphoric acid esters affect the kinetic parameters of the aerosol, which were obtained on the basis of mathematical calculation. Diethyl phosphite produces the greatest effect on the decrease in the aerosol's stability. The formation of an aerosol having a smaller particle size occurs during thermal decomposition of the modified wood having a thermally stable surface. Therefore, the modification of wood by phosphoric acid esters reduces its propensity to smoke-generating ability, which determines the reduction in death rate of humans in the event of fire.

1. Foreword

According to Federal Law No. 123 "On fire safety requirements", the reduced visibility on evacuation routes and toxicity of thermal decomposition products refer to dangerous fire factors. The possibility of exposure to these hazards is determined by the formation of smoke during the thermal decomposition of combustible construction materials. Smoke is an aerosol produced by the thermal decomposition of materials. Based on the example of wood as a widespread construction material [1-2], the formation of aerosols can be characterized as follows. When exposed to high temperatures (from 350 °C), the wood composite decomposes releasing combustible gaseous substances and chemical decomposition processes in the solid phase [3-4] take place. In addition to the above, a surface coking layer is formed, which depending on the material properties and the intensity of the thermal effect can be characterized



by different porosity and diffusion resistance. The highest degree of smoke emission is observed in the flameless thermal decomposition – smouldering, at a temperature of 350-450 °C.

In the event of a fire, the danger of smoke is caused by panic and disorientation of a person in dangerous conditions, as well as by the deterioration of the operating conditions of rescue teams. A number of studies in the field of people's behaviour in dangerous situations [5-11] have shown that with a reduced visibility on evacuation routes, people are reluctant to leave temporarily safe premises (except for the rooms where a fire has occurred). This may be the reason of cutting off people from the building exits and their evacuation may result in additional casualties. Staying in a smoke-filled room can cause respiratory diseases and pathologies due to inhalation of thermal decomposition toxic products.

At the present time, the influence of the wood species on the properties of fumes has been studied [12-14]. In addition, the influence of wood modification on the smoke-forming ability has been considered. Of particular importance in this matter is surface adsorption and chemical modification as an effective method for improving the properties of wood materials and reducing smoke formation [15]. The issue of the effect on structure and properties of the smoke aerosol is little studied. Detailed study of this issue is relevant for ensuring the safety of people in the event of a fire.

With reference to the foregoing, the work objective is to evaluate the effect of the wood surface layer modifiers on the formation and stability of smoke aerosols. To do this, it is necessary to cope with the following tasks: determination of the quantitative characteristics of the smoke aerosols formed during thermal decomposition of the original wood and modified wood, and also assessment of the effect of modifiers on the structure and properties of the surface layer of wood during its thermal decomposition.

2. Materials and methods

To assess the quantitative characteristics of the aerosol, granulometric analysis was performed using a Laser diffraction particle sizing analyser Cilas 1180. Coagulation of particles occurred during the aerosol formation and deposition. To reverse this effect, the deposited particles were placed in a 50% solution of isopropanol in water and subjected to ultrasonic treatment before and during the tests.

The smoke-forming ability was assessed using the smoke-forming coefficient determination apparatus in accordance with GOST 12.1.044 – 89 cl. 4.18

To study the efficiency of surface adsorption and chemical modification, an ultimate analysis was performed using Quanta 200 scanning microscope.

To assess the energy properties of the surface of modified wood samples, a neutral drop method was used to determine the surface tension of the samples and the nitrogen vapour sorption method was applied with the use of Quantachrome NOVA 4200e unit to estimate the specific area of the samples. To carry out the research, the samples of the deposited aerosol particles of the smoke formed during the thermal decomposition of the modified wood were used.

20% solutions of phosphoric acid esters: dimethyl phosphite (DMP), diethyl phosphite (DEP), dibutyl phosphite (DBP), diphenyl phosphite (DPP), ammonium polyphosphate (APP-1) were used as the wood surface layer modifiers. These modifiers were selected based on the fact that phosphoric acid esters refer to modifiers that reduce flammability and increase the biological stability of wood. Surface modification of wood took place under mild conditions (200 °C, 1 atm) at a consumption of compositions equal to 200 g/m². Combustion of modified wood was carried out in a special combustion chamber under smouldering conditions (T = 450 °C). The resulting smoke entered a special chamber in which deposition occurred within 24 hours.

3. Results and discussions

As a result of the granulometric measurements, the size distribution of particles of the smoke aerosol solid phase depending on the wood surface layer modifier (Table 1) was determined.

Table 1. Particle size distribution of aerosol disperse phase

r, μm	Original wood	Wood modified by				
		DFF	DBF	DMF	PFA-1	DEP
0.04–0.30	0.29	0.29	0.33	1.23	0.99	0.76
0.4	0.18	0.24	0.24	0.52	0.95	0.90
0.5	0.24	0.36	0.39	0.59	1.78	1.50
0.6	0.46	1.55	0.61	0.65	1.96	1.82
0.7	0.75	0.89	0.45	1.05	2.37	2.21
0.8	1.16	1.12	1.02	1.57	2.26	2.24
0.9	1.37	1.25	1.13	1.85	2.21	2.43
1.0	1.5	1.39	1.25	2.00	2.35	2.31
1.1	1.57	1.41	1.12	2.06	2.42	2.20
1.2	1.60	1.51	1.36	2.09	2.55	1.94
1.3	1.60	1.55	1.45	2.11	2.59	1.95
1.4	1.61	1.52	1.61	2.11	2.45	1.99
1.6	1.57	1.45	1.57	2.07	2.43	2.52
1.8	1.53	1.40	1.53	2.03	2.49	2.69
2.0	1.47	1.41	1.47	1.96	2.55	2.85
2.2	1.39	1.55	1.68	1.88	2.65	2.93
2.4	1.39	1.67	2.45	1.91	2.68	3.19
2.6	1.46	2.01	3.12	1.97	2.70	3.32
3.0	1.64	2.45	3.56	2.19	2.72	3.62
4.0	2.32	2.86	4.07	2.88	3.01	3.96
5.0	3.26	3.01	4.48	3.51	3.05	4.28
6.0	3.69	3.36	4.65	3.56	3.29	4.41
6.5	3.75	3.41	4.21	3.29	3.73	4.52
7.0	3.73	3.51	3.73	3.25	3.95	5.08
7.5	3.76	3.45	3.76	3.30	4.65	5.38
8.0	3.79	3.36	3.80	3.51	5.15	5.33
8.5	3.86	3.54	3.75	3.84	5.41	5.03
9.0	4.06	3.96	4.06	4.25	5.05	4.73
10.0	4.53	4.12	4.89	5.99	4.86	4.21
11.0	5.12	4.51	5.75	5.85	4.22	3.67
12.0	5.31	4.89	5.25	5.35	3.62	3.21
13.0	5.52	5.01	5.12	5.12	2.86	2.08
14.0	5.65	5.13	4.23	4.45	2.09	0.53
15.0	5.01	4.85	3.54	3.60	1.29	0.21
16.0	4.08	4.25	3.11	2.73	0.59	–
17.0	3.32	3.78	2.15	2.02	0.13	–
18.0	2.60	3.15	1.56	1.15	0.05	–
19.0	1.80	2.58	1.12	0.46	–	–
20.0	1.25	1.54	0.36	0.05	–	–
22.0	0.70	0.59	0.07	–	–	–
25.0	0.11	0.12	–	–	–	–

According to the data obtained, it can be seen that the wood surface layer modifiers produce a significant impact on the quantitative characteristics of the smoke aerosols formed during the thermal decomposition of the modified wood. The maximum particle size of the particulate disperse phase of the smoke aerosol produced by the thermal decomposition of the original wood is 25 μm . When DMPs are used as modifiers, the maximum particle size is 20 μm , for APP-1 it is 18 μm and for DEP it is 15 μm . This significantly impacts the optical characteristics of smoke. According to the results of tests for determining the smoke-generating index, the maximum smoke-generating capacity is peculiar to the original wood, whereas in the case of using the chosen modifiers, a significant reduction in smoke generation occurs. DEP is the most effective modifier (Table 2).

Table 2. The smoke-generating capacity of the original and modified wood

	Original wood	Wood modified by				
		DMF	DEP	DFP	DBF	PFA-1
$D_m, \text{m}^2/\text{kg}$	1100	510	160	740	600	440

To form a strong and stable structure of the surface layer of wood, it is necessary to obtain strong covalent bonds between the modifier and the components of the lignin-carbohydrate complex of wood. The quantitative characteristics of chemical modification are determined based on the percentage of phosphorus in the modified wood surface layer. The character of the thermal decomposition of the wood modified by phosphorous-containing organic compounds is influenced by the formation parameters and the structure of the coking layer. The phosphorous-containing structure is the most stable structure of coke. The most effective modifier is DEP, which is highly resistant to the thermal decomposition of wood modified with this modifier (Table 3).

Table 3. The phosphorous content in the surface layer of wood before and after thermal decomposition

Condition of wood	Phosphorus contents in wood modified by, %				
	DMF	DEP	DBF	DFP	PFA-1
Before thermal decomposition	2.87	3.57	2.65	2.45	2.11
After thermal decomposition	0.85	4.70	0.71	1.06	0.35

To assess the stability of aerosols, it is necessary to determine their kinetic parameters: the coagulation rate and the sedimentation rate, which are determined by the structure of the solid particles of the dispersed phase and the Brownian motion [16-21]. Sedimentation rate is determined by the equation:

$$W_g = \frac{2r^2 \cdot \rho_z \cdot g}{9\mu} \quad (1)$$

where r is the radius of the solid particles of the disperse phase of the aerosols, ρ is the particle density, g is the gravity acceleration, μ is the medium viscosity ($\mu = 1.81 \cdot 10^{-4} \text{ Pa}\cdot\text{s}$).

Relying on the Brownian motion, the coagulation rate is expressed by the equation:

$$\frac{dN}{dt} = \frac{4K \cdot T}{3\mu} \left(1 + \frac{A \cdot l}{r}\right) N^2 \quad (2)$$

where N is the number of particles with a radius, A is the Stokes-Cunningham correction factor, K is the Boltzmann constant, T is the ambient temperature ($T = 70 \text{ }^\circ\text{C}$), l is the free length of molecule ($l = 65.3 \text{ nm}$). The number of particles of the solid aerosol disperse phase was obtained based on the mass of the solid aerosol disperse phase and the particle size distribution. The results of calculating the aerosol kinetic parameters are presented in Table 4.

Depending on the modifier of the wood surface layer, a change in the coagulation rate is observed. For particles with a radius of $0.2 \text{ }\mu\text{m}$, the coagulation rate increases with the use of DMP and DEP (falls by 3-4 times). When DPP and DBP are used, the coagulation rate changes insignificantly, which is determined by the nature of the modifiers in the phosphoryl group. APP-1 is a salt component, which when used allows rapid coagulation of small particles and a low coagulation rate of large particles. The coagulation rate is determined by the number of particles. With the increase in the radius of particles, the rate of their coagulation with the use of DEP is significantly reduced, which is related to the small

concentration of large-sized particles and the smallest total mass of aerosol particles formed during the thermal decomposition of the DEP-modified wood.

Table 4. Sedimentation rate and coagulation rate of aerosol solids

R, μm	W_g , m/s	The speed of the coagulation of aerosol particulate matter during combustion of					
		original wood	wood modified by				
			DMF	DEP	DFE	DBF	PFA-1
0.2	$2.16 \cdot 10^{-7}$	$1.40 \cdot 10^{-8}$	$3.17 \cdot 10^{-8}$	$5.76 \cdot 10^{-8}$	$1.10 \cdot 10^{-8}$	$2.0 \cdot 10^{-8}$	$1.6 \cdot 10^{-7}$
3.0	$4.87 \cdot 10^{-5}$	$1.51 \cdot 10^{-10}$	$2.69 \cdot 10^{-10}$	$2.67 \cdot 10^{-10}$	$3.80 \cdot 10^{-10}$	$1.0 \cdot 10^{-9}$	$3.9 \cdot 10^{-10}$
10.0	$5.40 \cdot 10^{-4}$	$9.16 \cdot 10^{-12}$	$1.10 \cdot 10^{-11}$	$5.20 \cdot 10^{-12}$	$8.50 \cdot 10^{-12}$	$1.5 \cdot 10^{-11}$	$1.0 \cdot 10^{-11}$
15.0	$1.20 \cdot 10^{-3}$	$1.99 \cdot 10^{-12}$	$1.14 \cdot 10^{-12}$	$1.70 \cdot 10^{-15}$	$2.34 \cdot 10^{-12}$	$1.5 \cdot 10^{-12}$	$1.4 \cdot 10^{-13}$
Δm , g		2.60	2.30	1.55	2.45	2.74	2.25

To investigate the principle of the smoke suppressing action of modifiers, a study of the properties of the surface layer of modified wood and its change due to thermal decomposition based on the energy characteristics of the surface of the modified wood before and after thermal decomposition was carried out. Using the combined equation, I-II of thermodynamics laws (3), a change in the Gibbs thermodynamic potential was calculated [22-24]:

$$\Delta G = \sigma dS_{sp} + S_{sp} d\sigma \quad (3)$$

where σ is the surface tension of the sample, S_{sp} is the specific surface area. The data obtained from the tests and calculations are presented in Table 5.

Table 5. Energy characteristics of the modified wood surface

	Original wood	Wood modified by				
		DMF	DEP	DFE	DBF	PFA-1
$\sigma_c \cdot 10^3$, N/m	25.33/16.71	19.91/19.07	25.03/24.06	23.03/19.07	22.36/17.36	20.05/22.24
ΔG , kJ	-	-12.68/14.31	-14.5/-14.48	-10.16/-13.69	-6.97/2.43	-2.71/12.35

^a Note: Above the line are data for wood before thermal decomposition, under the line is after it.

The data obtained show that the surface of a wood sample modified by DEP has the greatest stability during thermal decomposition, since it has the greatest values of surface tension, and the deviations ΔG before and after thermal decomposition are close to zero.

4. Conclusions

The kinetic parameters of sedimentation and coagulation of aerosols formed during the thermal decomposition of modified wood depend on the nature of modifier. In the series of phosphoric acid esters, the best modifier is DEP, which causes the highest destruction rate of the smoke aerosol. The modifier's nature affects the properties of the wood surface. When modifying takes place, an increase in surface tension occurs. A change in the Gibbs thermodynamic potential characterizes the stability of the modified surface. It is quantitatively determined by the total mass of the solid particles of the smoke aerosol disperse phase, and also by the decrease in the maximum diameter of the particles. Therefore, the modification of wood by phosphoric acid esters reduces its propensity to smoke-generating ability, which determines the reduction in death rate of humans in the event of fire.

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