

Original Research

Reducing Concentrations of Benzo(a)pyrene in Gas Phase Soot Particles by Using and Burning Water Fuel Emulsions

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Received: 23 July 2019

Accepted: 15 September 2019

Abstract

In this study, benzo(a)pyrene-water-oxygen systems were investigated in wide ranges of change of temperature value and initial components to predict in which conditions benzo(a)pyrene degraded into more harmful substances. Consequently, the thermodynamic parameters of the benzo(a)pyrene-water-oxygen system were calculated and the concentration distribution of carbon, hydrogen and oxygen-containing particles in the gas phase were established. Adding water into the system allowed decreasing of carbon and acetylene. These elements are the key elements of benzo(a)pyrene formation. According to this, the main parameter for reducing the concentration of benzo(a)pyrene in the gas phase was the water content in fuel oil within 10-15%.

Determination of the concentration of benzo(a)pyrene in samples of flue gases of DKVR-4/13 and PTVM- 30M boiler units of the Teplokommunoenergo heating organization of Bishkek city was carried out by chromatographic method. Concentrations of benzo(a)pyrene were found to compare the product of burning ordinary fuel oil and water fuel emulsion. Homogenization of the fuel-air mixture by adding water to the fuel oil allowed us to obtain an inverse emulsion and reduce the concentration of benzo(a)pyrene in flue gases up to 62%. According to this, a new process flowsheet of water fuel emulsions production was proposed for the heating organization.

Keywords: Benzo(a)pyrene, PAH, carcinogenic pollutants, soot, combustion processes

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Introduction

Pyrolysis of organic fuels in a gaseous phase leads to the release of a wide class of unburned hydrocarbons, and furthermore, in the combustion process heavier hydrocarbons such as polycyclic aromatic hydrocarbons (PAH) can be synthesized [1], which are able to group the benzene ring compound [2-6]. Generally, the formation of benzo(a)pyrene occurs in two main ways. It forms as a result of condensation of benzene rings [3] as well as during the decomposition of aromatic compounds into lighter ones and their further polymerization at high temperatures. The key element in the formation of benzo(a)pyrene is the propargyl radical (C_3H_3), where two radicals form an aromatic ring. Benzo(a)pyrene is an intermediate fragment in the formation of condensed carbon as well, consequently, $C_{20}H_{12}$ during the formation process is adsorbed on the soot particles of flue gases and is gradually dispersed in the surrounding natural environment [7]. It especially occurs in the winter during heating periods [8-11].

In terms of environmental impact, the entire class of hydrocarbons are related to pollutants. A special place in this class is taken by benzo(a)pyrene ($C_{20}H_{12}$), since benzo(a)pyrene (as well as some other PAHs) might cause cancer in living organisms and cell mutation [12, 13]. According to this, maximum exposure limit

(MEL) and occupational exposure limit (OEL) are many times tougher than for any other hydrocarbon groups. Moreover, benzo(a)pyrene is proposed as an indicator for the carcinogenic fraction of these PAHs [14-16]. Getting into an organism of single PAH compounds, for example benzo(a)pyrene alone, does not occur without other PAHs being present [17].

Consequently, safety problems related to benzo(a)pyrene continue to remain actual and the development of effective ways to minimize benzo(a)pyrene in a technogenic environment is still unresolved [18-27]. Therefore, in this study the formation and degradation of benzo(a)pyrene in model conditions was calculated according to thermodynamic conditions. The prediction of the reaction kinetics of PAHs requires an accurate description of their thermochemical properties. Accordingly, physico-chemical modeling of the thermal degradation of benzo(a)pyrene in a wide range of temperature change of conversion medium, prediction and reduction concentration of toxic substances in the gas phase is an actual scientific challenge.

Material and Methods

In this study, thermodynamic data were used in order to simulate the benz(a)pyrene-oxygen-water

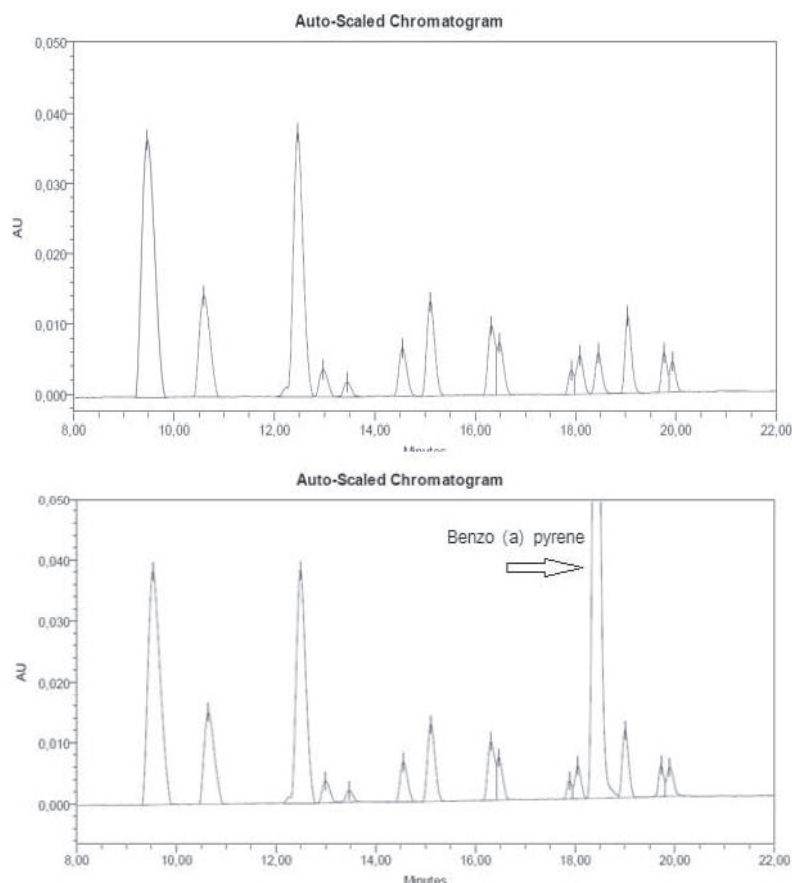


Fig. 1. Chromatogram of soot spiked with standard benzo(a)pyrene.

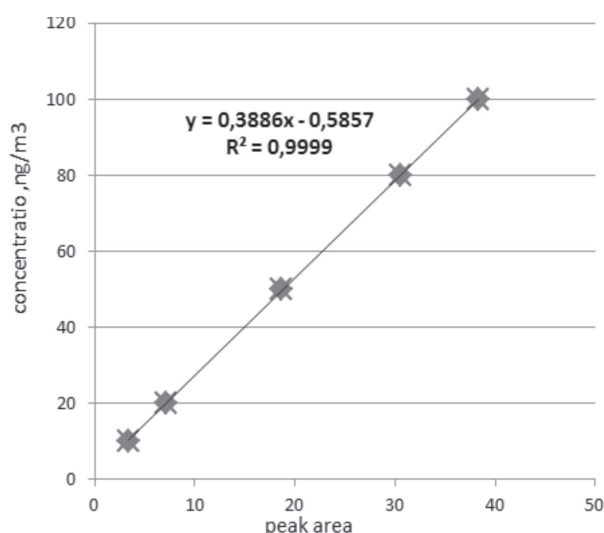


Fig. 2. Concentration of $C_{20}H_{12}$ versus peak area.

systems with the Terra software package program [28, 29], based on the principle of maximum entropy, which provided information on the energy and concentration characteristics of the components in a wide range of pressure (P, MPa) and temperature (T, K) change.

Identification and quantitative analysis of benzo(a)pyrene were performed by Waters 2690 Separations Module high-performance liquid chromatography (HPLC) with a Shimadzu RF 551 fluorometric detector using a Phenomenex C18 column (250×46 mm). The column temperature was 25°C. Injected sample volume was 25 μ L. As a mobile phase, 60% acetonitrile and 40% water were used with a linear gradient to 100% acetonitrile. The flow rate was 1 mL/min. The data were collected and processed using the Waters Alliance Chemstation software and hardware complex [26, 29-33].

The determined peak of benzo(a)pyrene by adding a standard solution into the sample is shown in Fig. 1. Standard solutions for calibration were prepared and the peak area of each of them were obtained. The calibration

curve was prepared using a relationship between the concentration of standard solution of benzo(a)pyrene and the chromatographic peak area (Fig. 2). Obtained linear equation was $y = 0.3886x - 0.5857$, where y is the concentration of benzo(a)pyrene (ng/m³) and x is the peak area. The correlation coefficient (R^2) was 0.9999 [29].

Results and Discussion

Benzo(a)pyrene-oxygen, benzo(a)pyrene-water, and benzo(a)pyrene-water-oxygen systems were studied at the entropy maximum. The thermodynamic parameters of the benzo(a)pyrene-water-oxygen system (Table 1) were calculated and it was shown that the values of total enthalpy ($\Delta I < 0$) and internal energy ($\Delta U < 0$) were negative, which indicates that process of benzo(a)pyrene destruction occurs with the formation of low molecular weight components and particles (Table 2). The Prandtl number (Pr) identifies the ratio of kinematic viscosity to the diffusion coefficient in the gas phase (Table 1), which varies from 0.16 to 0.66 (according to the theory of gas dynamics $Pr < 1$). The adding of water into the $C_{20}H_{12}$ -O₂ system led to a radical decrease in condensed carbon (C) in the gas phase (Fig. 3): $C = 13,5602$ mol/kg at 500 K; $C = 1 \cdot 10^{-30}$ mol/kg at 2000 K. Accordingly, the formation of condensed carbon and acetylene is practically not observed in $C_{20}H_{12}$ - H₂O - O₂ (1:10:1) system (Fig. 4, Table 3).

Table 2 shows the main products of the conversion of benzo(a)pyrene in the gas phase: H, H₂, OH, H₂O, O, O₂, C, CO, CO₂, CH₄. Considering that polycyclic aromatic hydrocarbons (including benzo(a)pyrene) as one of the stages of the formation of soot, aromatic hydrocarbons convert into carbon black during combustion by direct condensation. Also, acetylene plays an important role (Table 3): $C_2H_2 = 4.05 \cdot 10^{-22}$ mol/kg at 500 K; $6.16 \cdot 10^{-9}$, 1000 K; $3.77 \cdot 10^{-10}$, 1500 K; $1.03 \cdot 10^{-10}$, 2000 K; $5.04 \cdot 10^{-11}$, 2500 K), as one of

Table 1. Change features of $C_{20}H_{12}$ -H₂O-O₂ (1:10:1) system, P = 0.1 MPa, T = 500-2500 K.

T. K	$V \cdot 10^2, m^3/kg$	S. kJ/(kg·K)	I. kJ/kg	U. kJ/kg	$C_p \cdot 10^4, kJ/(kg \cdot K)$	$\mu \cdot 10^5, Pa \cdot s$	$Lt' \cdot 10^5, W/(m \cdot K)$	$Pr' \cdot 10^3$
500	208.1	10.6	-11889.2	-11973.3	22103.5	1.8	24183.9	165.0
750	337.8	12.0	-11021.1	-11224.7	36633.9	2.7	85177.4	118.6
1000	455.9	12.7	-10392.8	-10712.8	23477.7	3.5	13301.5	629.0
1250	569.9	13.2	-9791.1	-10225.2	24594.9	4.2	16574.3	635.7
1500	683.9	13.7	-9164.4	-9712.5	25531.9	4.9	19815.5	637.7
1750	798.0	14.1	-8514.1	-9176.2	26525.7	5.5	23030.7	641.7
2000	912.4	14.5	-7833.2	-8609.6	28163.3	6.1	26205.9	661.9
2250	1028.6	14.8	-7083.2	-7975.6	32686.0	6.7	41206.2	532.7
2500	1153.3	15.2	-6114.3	-7130.1	47771.2	7.2	83766.3	413.4

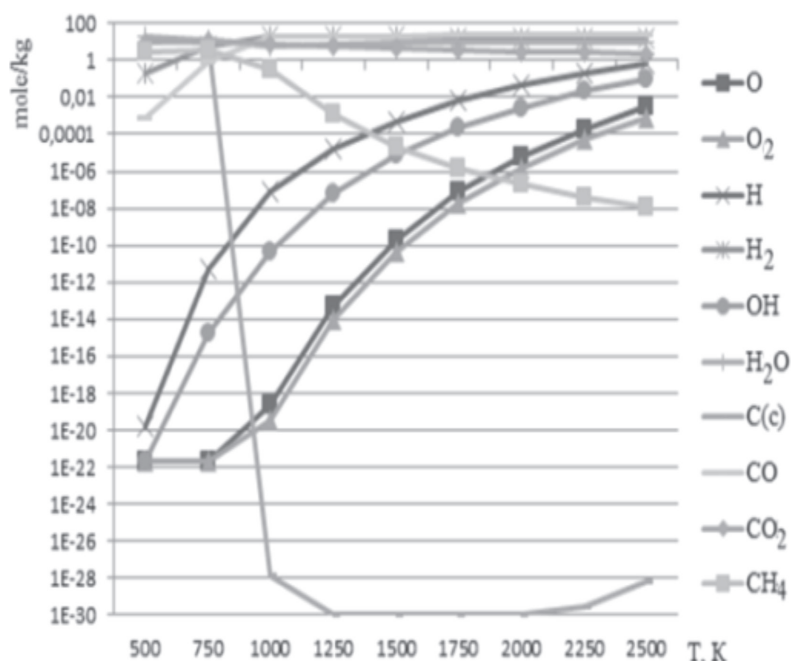


Fig. 3. Equilibrium composition and concentration of components, which occurs in the $C_{20}H_{12}-H_2O-O_2$ (1:1:1) system.

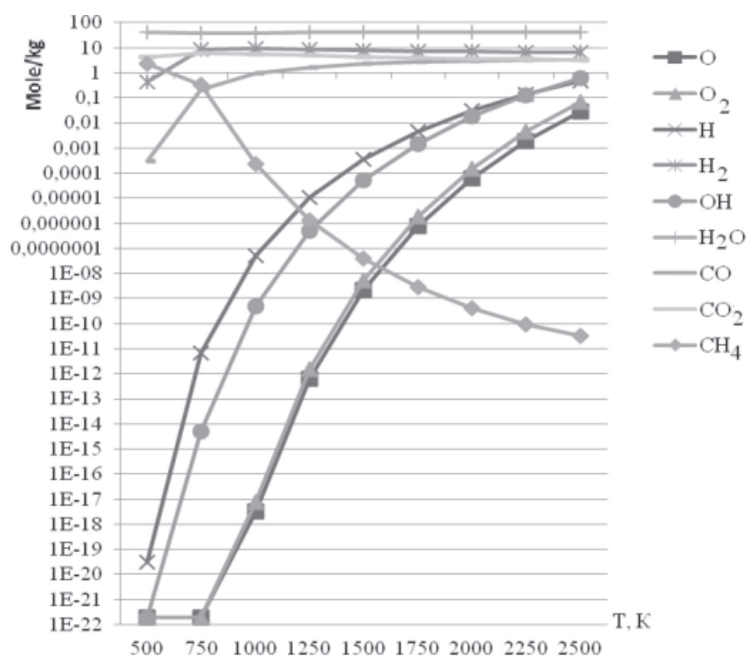


Fig. 4. Equilibrium composition and concentration of components, which occurs in the $C_{20}H_{12}-H_2O-O_2$ (1:10:1) system.

the main elements included in the kinetic schemes for the synthesis of aromatic hydrocarbons.

Chemical mechanisms of soot formation using aromatic hydrocarbons containing fuels, the synthesis of benzo(a)pyrene comes in two ways: by condensation of benzene rings, and by polymerizing the pyrolysis products. In the second case, an important role is played by acetylene (mol/kg) as one of the main elements included in the kinetic scheme of synthesis of aromatic hydrocarbons [1, 6, 34-36]

Research on the mechanism of formation of benzo(a)pyrene during burning previously prepared water fuel emulsions showed that the level of concentration of the substance depends on the type of fuel mixture composition and the intensity of diffusion processes in the combustion zone [6, 8, 21, 37, 38]. For a given type of fuel, the main determining parameter was the mixture composition, which was characterized by excess air coefficient and the amount of water in the fuel [39-45].

Table 2. Equilibrium composition and concentration of components (mol/kg), which occurs in the $C_{20}H_{12}-H_2O-O_2$ (1:10:1) system, $P = 0.1$ MPa, $T = 500-2500$ K.

Composition	Temperature, K								
	500	750	1000	1250	1500	1750	2000	2250	2500
O	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$3.2 \cdot 10^{-18}$	$6.2 \cdot 10^{-13}$	$2.1 \cdot 10^{-9}$	$7.5 \cdot 10^{-7}$	$6.1 \cdot 10^{-5}$	$1.8 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$
O ₂	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$7.7 \cdot 10^{-18}$	$1.4 \cdot 10^{-12}$	$5.2 \cdot 10^{-9}$	$1.8 \cdot 10^{-6}$	$1.5 \cdot 10^{-4}$	$4.7 \cdot 10^{-3}$	$6.8 \cdot 10^{-2}$
H	$3.2 \cdot 10^{-20}$	$6.7 \cdot 10^{-12}$	$5.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-5}$	$3.6 \cdot 10^{-4}$	$4.6 \cdot 10^{-3}$	$3.2 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$4.9 \cdot 10^{-1}$
H ₂	0.4	8.4	9.0	8.3	7.7	7.3	7.0	6.8	6.8
OH	$1.9 \cdot 10^{-22}$	$5.2 \cdot 10^{-15}$	$4.8 \cdot 10^{-10}$	$5.0 \cdot 10^{-7}$	$5.3 \cdot 10^{-5}$	$1.5 \cdot 10^{-3}$	$1.8 \cdot 10^{-2}$	$1.2 \cdot 10^{-1}$	$6.0 \cdot 10^{-1}$
HO ₂	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$4.5 \cdot 10^{-21}$	$9.6 \cdot 10^{-16}$	$3.6 \cdot 10^{-12}$	$1.3 \cdot 10^{-9}$	$1.1 \cdot 10^{-7}$	$3.5 \cdot 10^{-6}$	$5.2 \cdot 10^{-5}$
H ₂ O	43	39	39	39	40	40	41	41	40
H ₂ O ₂	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$4.2 \cdot 10^{-17}$	$2.4 \cdot 10^{-13}$	$8.3 \cdot 10^{-11}$	$5.4 \cdot 10^{-9}$	$1.2 \cdot 10^{-7}$	$1.5 \cdot 10^{-6}$	$1.0 \cdot 10^{-5}$
C	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.2 \cdot 10^{-20}$	$1.1 \cdot 10^{-17}$	$1.8 \cdot 10^{-15}$	$9.3 \cdot 10^{-14}$	$2.3 \cdot 10^{-12}$
CO	$3.0 \cdot 10^{-4}$	0.21	0.91	1.6	2.2	2.6	2.9	3.1	3.3
CO ₂	4.2	6.0	5.6	4.9	4.4	3.9	3.6	3.4	3.2
CH	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$3.0 \cdot 10^{-19}$	$6.4 \cdot 10^{-17}$	$3.4 \cdot 10^{-15}$	$7.7 \cdot 10^{-14}$	$9.7 \cdot 10^{-13}$
CH ₂	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$4.2 \cdot 10^{-20}$	$2.4 \cdot 10^{-17}$	$1.4 \cdot 10^{-15}$	$2.6 \cdot 10^{-14}$	$2.2 \cdot 10^{-13}$	$1.1 \cdot 10^{-12}$	$4.6 \cdot 10^{-12}$
CH ₃	$1.7 \cdot 10^{-18}$	$3.8 \cdot 10^{-12}$	$2.2 \cdot 10^{-11}$	$3.3 \cdot 10^{-11}$	$3.7 \cdot 10^{-11}$	$3.8 \cdot 10^{-11}$	$3.8 \cdot 10^{-11}$	$3.8 \cdot 10^{-11}$	$4.1 \cdot 10^{-11}$
CH ₄	2.3	$3.0 \cdot 10^{-1}$	$2.2 \cdot 10^{-4}$	$1.3 \cdot 10^{-6}$	$3.8 \cdot 10^{-8}$	$2.9 \cdot 10^{-9}$	$4.2 \cdot 10^{-10}$	$9.6 \cdot 10^{-11}$	$3.2 \cdot 10^{-11}$
C ₂ H ₄	$8.9 \cdot 10^{-13}$	$9.7 \cdot 10^{-10}$	$2.1 \cdot 10^{-12}$	$1.6 \cdot 10^{-14}$	$5.1 \cdot 10^{-16}$	$3.9 \cdot 10^{-17}$	$5.6 \cdot 10^{-18}$	$1.2 \cdot 10^{-18}$	$4.2 \cdot 10^{-19}$
C ₂ H ₆	$5.1 \cdot 10^{-7}$	$1.2 \cdot 10^{-7}$	$9.6 \cdot 10^{-13}$	$2.2 \cdot 10^{-16}$	$6.4 \cdot 10^{-19}$	$9.0 \cdot 10^{-21}$	$3.6 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$
C ₃ H ₈	$1.2 \cdot 10^{-12}$	$2.4 \cdot 10^{-13}$	$1.4 \cdot 10^{-20}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$
CHO	$1.9 \cdot 10^{-22}$	$1.4 \cdot 10^{-14}$	$2.6 \cdot 10^{-11}$	$1.6 \cdot 10^{-9}$	$2.3 \cdot 10^{-8}$	$1.5 \cdot 10^{-7}$	$6.0 \cdot 10^{-7}$	$1.7 \cdot 10^{-6}$	$4.2 \cdot 10^{-6}$
CHO ₂	$1.8 \cdot 10^{-21}$	$1.8 \cdot 10^{-14}$	$2.3 \cdot 10^{-11}$	$1.4 \cdot 10^{-9}$	$2.0 \cdot 10^{-8}$	$1.4 \cdot 10^{-7}$	$5.8 \cdot 10^{-7}$	$1.7 \cdot 10^{-6}$	$4.2 \cdot 10^{-6}$
CH ₂ O	$2.3 \cdot 10^{-12}$	$2.3 \cdot 10^{-8}$	$8.6 \cdot 10^{-8}$	$1.2 \cdot 10^{-7}$	$1.4 \cdot 10^{-7}$	$1.5 \cdot 10^{-7}$	$1.5 \cdot 10^{-7}$	$1.6 \cdot 10^{-7}$	$1.7 \cdot 10^{-7}$
CH ₂ O ₂	$8.3 \cdot 10^{-9}$	$5.3 \cdot 10^{-7}$	$7.9 \cdot 10^{-7}$	$8.2 \cdot 10^{-7}$	$8.2 \cdot 10^{-7}$	$8.2 \cdot 10^{-7}$	$8.3 \cdot 10^{-7}$	$8.4 \cdot 10^{-7}$	$8.5 \cdot 10^{-7}$
CH ₃ O	$1.9 \cdot 10^{-22}$	$4.5 \cdot 10^{-20}$	$1.9 \cdot 10^{-17}$	$4.5 \cdot 10^{-16}$	$3.3 \cdot 10^{-15}$	$1.3 \cdot 10^{-14}$	$3.9 \cdot 10^{-14}$	$8.8 \cdot 10^{-14}$	$1.7 \cdot 10^{-13}$
C ₂ H ₄ O ₂	$2.7 \cdot 10^{-11}$	$8.8 \cdot 10^{-11}$	$2.5 \cdot 10^{-13}$	$3.5 \cdot 10^{-15}$	$1.8 \cdot 10^{-16}$	$2.1 \cdot 10^{-17}$	$4.2 \cdot 10^{-18}$	$1.2 \cdot 10^{-18}$	$4.7 \cdot 10^{-19}$
O ₃	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$6.8 \cdot 10^{-22}$	$5.5 \cdot 10^{-18}$	$6.2 \cdot 10^{-15}$	$1.6 \cdot 10^{-12}$

Table 3. Calculation of the concentration of carbon, hydrogen, and oxygen-containing particles (mol/kg) in the gas phase during the destruction of the benzo(a)pyrene-water-oxygen system; $P = 0.1$ MPa, $T = 500 - 2500$ K.

Systems	$C_{20}H_{12}-O_2$ (1:1)	$C_{20}H_{12}-H_2O$ (1:1)	$C_{20}H_{12}-H_2O-O_2$ (1:1:1)	$C_{20}H_{12}-H_2O-O_2$ (1:10:1)
H ₂	$8 \cdot 10^{-2}$ —11	0.3—38	0.2—15	0.4—6.8
H	$9.2 \cdot 10^{-21}$ —0.5	$2.4 \cdot 10^{-20}$ —1.2	$1.8 \cdot 10^{-20}$ —0.7	$3.2 \cdot 10^{-20}$ —0.4
CO	$6.0 \cdot 10^{-4}$ —31	$4 \cdot 10^{-4}$ —27	$7 \cdot 10^{-4}$ —23	$3 \cdot 10^{-4}$ —3.3
CO ₂	10— $8.8 \cdot 10^{-5}$	3.5 — $4.4 \cdot 10^{-5}$	9.7—2.5	4.2—3.2
CH ₄	0.7 — $4 \cdot 10^{-4}$	9.3 — $3 \cdot 10^{-3}$	3.1 — $1.2 \cdot 10^{-8}$	2.3 — $3.2 \cdot 10^{-11}$
H ₂ O	10— $2 \cdot 10^{-4}$	20 — $3 \cdot 10^{-4}$	19—10	43—40
C ₂ H ₂	$1.9 \cdot 10^{-22}$ —0.1	$7 \cdot 10^{-22}$ —0.4	$4 \cdot 10^{-22}$ — $5 \cdot 10^{-11}$	—
C	28—8	26—10	13— $5.7 \cdot 10^{-29}$	—

Table 4. The ratio of atomic hydrogen-to-atomic carbon (H/C) in benzo(a)pyrene-containing systems; P = 0.1 MPa.

System	Composition, mol/kg	Temperature, K				
		500	1000	1500	2000	2500
$C_{20}H_{12} - O_2$ (1:1)	H/C	$9.2 \cdot 10^{-21}$	$4.2 \cdot 10^{-8}$	$3.9 \cdot 10^{-4}$	$3.6 \cdot 10^{-2}$	0.56
		$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$7.4 \cdot 10^{-16}$	$1.3 \cdot 10^{-9}$	$7.2 \cdot 10^{-6}$
$C_{20}H_{12} - H_2O - O_2$ (1:10:1)	H/C	$3.2 \cdot 10^{-20}$	$5.1 \cdot 10^{-8}$	$3.6 \cdot 10^{-4}$	$3.2 \cdot 10^{-2}$	0.49
		$1.9 \cdot 10^{-22}$	$1.9 \cdot 10^{-22}$	$1.3 \cdot 10^{-20}$	$1.8 \cdot 10^{-15}$	$2.3 \cdot 10^{-12}$

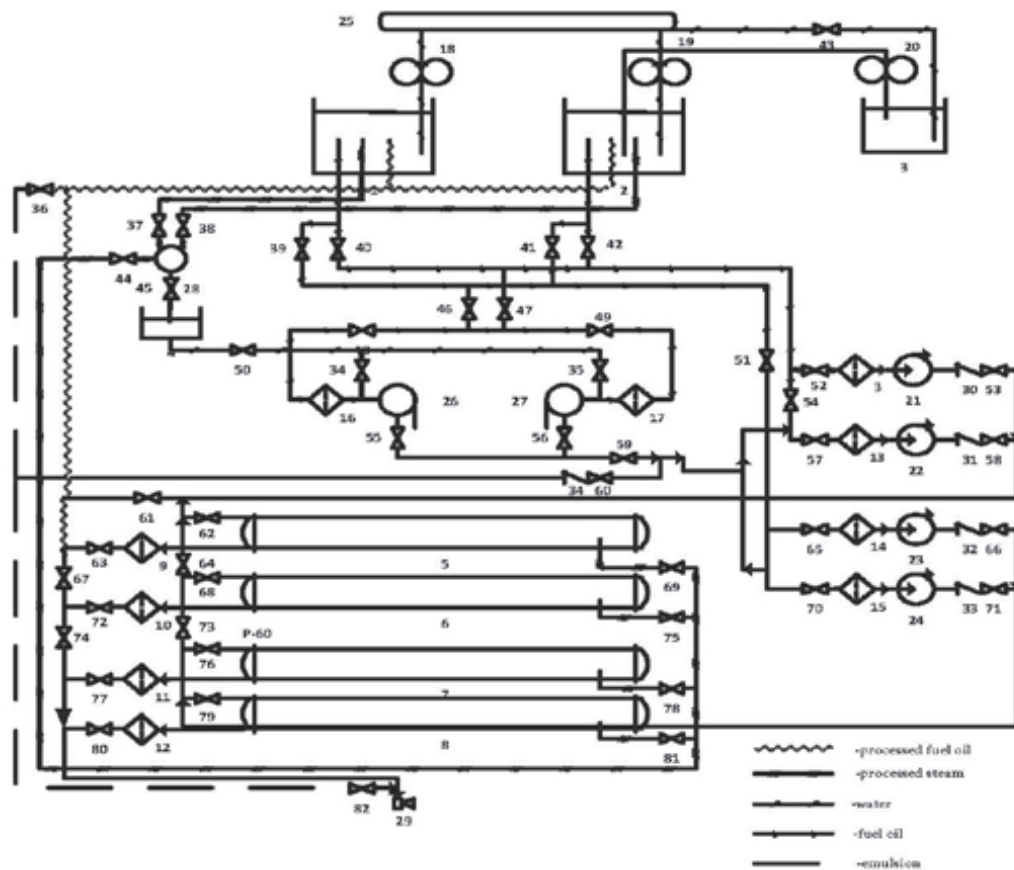


Fig. 5. Process flowsheet for the preparation and burning of water fuel emulsion in boilers of the type DKVR - 4/13 and PTVM - 30M: 1, 2 - tanks V = 500 m³, 3 - pumped water tank, 4 - working water tank, 5-8 - heat exchangers, 9-17 - coarse filters, 18-19 - pumps for water pumping, 20 - pump for pumping fuel oil, 21-24 - working pumps, 25 - water collector, 26-27 - rotary pulsation apparatus, 28 - exhaust steam cooler, 29 - boiler nozzles, 30-34 - check valves, 34-35 - valves, and 36-81 – latches.

Table 5. Reduction of pollutant concentrations in the gas phase.

Gas emission components	Concentrations of harmful substances emitted into the atmosphere, mg/m ³					
	DKVR -4/13			PTVM-30M		
	Fuel oil	Water fuel emulsion	Decreasing, %	Fuel oil	Water fuel emulsion	Decreasing, %
Sulfur dioxide	372	352	5.3	341	320	6.1
Nitrogen oxides	112	47	58	108	44	59.2
Carbon monoxide	310	140	54.8	295	125	57.8
Hydrocarbon oil	420	200	52.3	320	150	53.1
Soot	55	21	61.1	30	14	53.3

Table 6. Reduction of benzo(a)pyrene concentrations in the gas phase.

The concentration of benzo(a)pyrene	Type of fuel	Boiler Units	
		PTVM- 30M	DKVR-4/13
$C_{20}H_{12}$, 10^{-5} , mg/m ³	Fuel oil	38.5	31.5
$C_{20}H_{12}$, 10^{-6} , ton/year		280.1	24.8
$C_{20}H_{12}$, 10^{-5} , mg/m ³	Water fuel emulsion	18.0	12.0
$C_{20}H_{12}$, 10^{-6} , ton/year		130.7	9.4
Decreasing of $C_{20}H_{12}$ in gas phase, %		53.2	62.0

The reducing effect of water on the formation of benzo(a)pyrene in the gas phase was used in DKVR-4/13 and PTVM-30-type boiler units, Teplokommunoenergo, Bishkek city, by modifying fuel oil into water fuel emulsions [45, 46]. The main parameter of reducing the concentration of benzo(a)pyrene in the gas phase was water content in the fuel oil in the range of 10-15%.

The homogenization and obtaining an inverse emulsion of the fuel-air mixture can significantly reduce the concentration of benzo(a)pyrene by creating cavitation effects based on the rotary pulsation apparatus [47], while polydisperse water fuel emulsions are obtained according to the developed process flowsheet shown in Fig. 5. Complete combustion of water fuel emulsions led to a radical decrease in the concentration of toxic substances (Table 5), including benzo(a)pyrene in the gas phase (Table 6).

Combustion of water fuel emulsions in DKVR-4/13, PTVM-30M boilers allowed for a reduction in the concentration of benzo(a)pyrene in the gas phase from 53 to 62% by creating developed contact surfaces of phases (Table 6).

Conclusions

Benzo(a)pyrene-oxygen, benzo(a)pyrene-water, benzo(a)pyrene-water-oxygen systems were studied at the entropy maximum. Equilibrium compositions and concentrations of components, particles and their distribution in the gas phase at different temperatures ($T = 500-2500$ K) and ratios of gas-liquid flows were established. Calculations showed that condensed carbon and acetylene were reduced or even not detected in the $C_{20}H_{12}$ - H_2O - O_2 (1:10:1) system due to the presence of a sufficient amount of hydrogen. Burning water fuel emulsions (90% fuel oil + 10% water) in small- and medium-capacity boilers reduced the benzo(a)pyrene content in soot particles of flue gases by about 62% by creating a developed contact surface of the interacting phases and total combustion of water fuel emulsions in the burning zone.

Conflict of Interest

The authors declare no conflict of interest.

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