Numerical research of heat and mass transfer at interaction of several hot particles with typical polymeric material

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Abstract. The results of numerical investigation of heat and mass transfer at polymeric material ignition by several small-size hot particles are presented. The developed mathematical model considers the thermal conduction in polymeric material and hot particles, thermal decomposition of condensed substance, diffusion and thermal convection of combustible gases in air. It has been determined that the joint effect of several local energy sources on the ignition delay time is absent when the distance between hot particles exceeds their characteristic size.

Keywords: hot particles, polymeric material, thermal conduction, thermal decomposition, diffusion, thermal convection, ignition, mathematical modeling.

1. Introduction
Dozens of large-scale fires occur every day at power plants, residential and public buildings. These incidents are very dangerous for human health. The fires consequences are characterized by high material losses. The large proportion of fires happens due to the interaction between small-sized hot particles and combustible substances (solid and liquid fuels, wood, polymers, etc.) [1–3]. Polymeric material products are used recently as a construction and decorative elements in industrial, public and residential buildings. These products have shortcomings: variation of the strength characteristics, a high fire hazard and a toxicity of pyrolysis products emitted under heating.

Values of the main integral characteristics [4,5] were determined as a result of the numerical investigations of polymeric materials (polystyrene, polymethyl methacrylate) ignition by the single hot particle. The formulated theoretical results can be applied for developing recommendations and measurements to prevent ignitions of polymeric materials products. In practice, as a rule, the fires occur at interaction between a group of particles heated to high temperatures and a condensed substance. The heat and mass transfer characteristics may be different at ignition process in the systems “single hot particle – polymeric material” and “group of hot particles – polymeric material". It is known that at high concentrations of hot particles per unit of combustible material surface the ignition delay time is close to the same characteristic for materials heating by a massive plate with a constant temperature. Therefore, the more detailed representations about the characteristics of physical and chemical processes during the induction period at the interaction between the polymeric material and the stream of particles are necessary for developing the preventive measures.

The purpose of the present work is the numerical investigation of the joint effect of several local energy sources heated to high temperatures on the integral characteristics of the polymeric material ignition, taking into account diffusion and thermal convection of combustible gases in the outside air.
2. Problem Statement

Characteristics and conditions of heat and mass transfer processes depend on the distance between two neighboring particles at different quantity of the hot particles located on the surface of condensed substance. Therefore investigation of ignition process was carried out in the system “two hot particles – polymeric material – air” (Figure 1).

As a result of the polymeric material near-surface layer (0<\(t\)<\(t_d\)) heating by the energy of the hot particles thermal decomposition of polymeric material occurred and combustible gases emitted to the outside air. The gaseous products of polymeric material pyrolysis mixed with the oxidant due to the diffusion and thermal convection in the air. The gas mixture was heated moving along the side faces of the energy sources (\(x=x_1, x=x_2, y_1<y<y_2\)). The gas-phase ignition in the system (Figure 1) happened at the critical values of the combustible component concentration and the gas mixture temperature.

![Figure 1. A scheme of the solution domain at t=0: 1 – air (gas mixture at 0<\(t\)<\(t_d\)), 2 – hot particle, 3 – polymeric material](image)

The assumptions were taken at the problem statement:

1. A contact between the energy sources and the polymeric material was ideal. A possible gas gap formation was not considered.
2. A possible burning out of polymeric material was not considered. Burning out of the near surface layer has an insignificant influence on the integral ignition characteristics under the local heating during short time period (less than 0.5 s).
3. As a result of polymeric material thermal decomposition only one gaseous substance with known thermal and kinetic characteristics was formed.

Ignition conditions [6]:

1. The energy released as a result of oxidation reaction of polymer material thermal decomposition products is more than the energy consumed by the hot particles to heating of a polymeric material and a gas mixture.
2. The temperature of a gas mixture in the zone of exothermic reaction exceeds the initial temperature of energy sources.


3. Mathematical Model and Solution Methods
To describe the interrelated physical and chemical processes in the system “two hot particles – polymeric material – air” (Figure 1) the mathematical model (non-stationary differential equations of mathematical physics in partial derivatives with corresponding initial and boundary conditions) was used [4,5]. It model takes into account heat and mass transfer at the conditions of chemical reaction.

At the solution of a system of differential equations the algorithm was used similar to the [4,5]. The system of equations with corresponding initial and boundary conditions was solved by the finite difference method. The alternating direction method was applied for solution the elliptical equations – continuity and motion. Difference analogues of energy and diffusion differential equations were solved by the locally one-dimensional method. The system of difference equations was solved by iteration method and sweep method at each iteration (for nonlinear equations) with using the implicit four-point difference scheme.

4. Results and Discussion
The numerical investigations of heat and mass transfer were carried out at interaction between hot steel particles in the form of parallelepiped with sizes \( x_p = 4 \times 10^{-3} \) m, \( y_p = 2 \times 10^{-3} \) m and polymethyl methacrylate (PMMA). An area with sizes \( x_L = 20 \times 10^{-3} \) m, \( y_L = 20 \times 10^{-3} \) m was selected in the polymeric material and air. The initial temperature of air and PMMA was \( T_0 = 300 \) K; the initial temperature of hot particles was varied in the range \( T_p = 700–1500 \) K. The distance between two neighboring particles is characterized by a dimensionless value \( L = \Delta x / x_p \). It varied in the range of \( L = 0.25–2 \).

Table 1 shows the ignition delay time \( t_d \) for PMMA at different values of \( L \) for the initial temperature \( T_p = 900 \) K of energy sources. It was established that in the system “two hot particles – polymeric material – air” the ignition delay time rose at increasing the distance between energy sources. At \( L > 1.5 \) the duration of investigated process does not change (\( t_d = 0.0939 \) s). This result is similar to the ignition delay time of PMMA by single hot particle (Table 2). Thus, the value of \( L = 1.5 \) is the limit (at \( T_p = 900 \) K). In this case the neighboring particles still have a joint effect on the intensity of heat and mass transfer processes.

| \( L \)     | 0.25 | 0.5  | 0.75 | 1   | 1.25 | 1.5  | 1.75 | 2   |
|------------|------|------|------|-----|------|------|------|-----|
| \( t_d, s \)| 0.0874 | 0.0915 | 0.0928 | 0.0934 | 0.0937 | 0.0939 | 0.0939 | 0.0939 |

At variation of distance between two neighboring particles the maximum change of ignition delay time in the system (Figure 1) is 6.7%. The joint influence of the hot particles on the intensity of heat and mass transfer processes decreases at the increasing initial temperature of energy sources.

The dependences of PMMA ignition delay time on the initial temperature \( t_d = f(T_p) \) of single particle and two particle at \( L = 0.25 \) are given in Table 2. It is shown that at \( T_p = 1150 \) K the values of ignition delay time are identical. This result can be explained by the fact that at increasing of \( T_p \) the heat content of energy sources rises and influence of neighboring particles on the polymeric material near-surface layer warming and gas mixture decreases. Therewith the temperature of the PMMA pyrolysis products increases, respectively, less time is required for warming up the mixture of combustible gases with an oxidant to the critical values. Ignition zones, as in the case of a single particle [4,5], are formed near the side faces of the local energy sources and shifted to the border “polymeric material – hot particle” (\( x = x_1, x = x_2, y \rightarrow y_1 \)).

| \( T_p, K \) | 700 | 800 | 900 | 1000 | 1100 | 1200 | 1300 | 1400 | 1500 |
|------------|-----|-----|-----|------|------|------|------|------|------|
| \( t_d^*, s \) | 0.2861 | 0.1506 | 0.0939 | 0.0685 | 0.0545 | 0.0462 | 0.0403 | 0.0358 | 0.0321 |
| \( t_d^{**, s} \) | 0.2317 | 0.1371 | 0.0874 | 0.064 | 0.0519 | 0.0462 | 0.0403 | 0.0358 | 0.0321 |

* – single particle.
** – two particles at \( L = 0.25 \).
Figure 2 shows the isotherms in the system (Figure 1) at the ignition moment at $T_p=900$ K for three different values of $L$.

Two ignition modes were found for the system “single hot particle – polymeric material – air” [4,5]. They are characterized by the position of oxidation reaction zone in the gas area near the hot particle in dependence on the initial temperature of local energy source. In this work two ignition modes were revealed too. They are characterized by the distance between two neighboring particles. The one local ignition zone (Figure 2 (a)) was formed at small value of $L=0.25$. This zone was situated on the symmetry axis of solution domain (Figure 1). As a result of joint effect of energy sources the maximum temperature gradients and the greatest concentration of PMMA pyrolysis products is in this area compared with the area $x>x_2$. At increasing of $L$ and another equal conditions (Figure 2 (b), (c)) two ignition zones were formed. Each of them was located in a small neighborhood of own energy source. At $L=0.25$ the concentration of polymeric material pyrolysis products is the same near the side faces of hot particles ($x=x_1$, $x=x_2$, $y_1<y<y_2$). However, the area of maximum temperature gradients was formed between the hot particles ($0<x<x_1$, $y_1<y<y_2$), where the ignition conditions were executed.

5. Conclusion
Numerical investigations carried out at the using of developed mathematical model of heat and mass transfer processes in the system “two hot particles – polymeric material – air” allowed to determine the maximum deviation of PMMA ignition delay time 12.3% (at $L=0.25$ and $T_p=700$ K) at polymeric material heating by a single hot particle and a group of hot particles. It means that analysis of the characteristics and laws of heat and mass transfer at the gas phase ignition of polymeric material by several small-sized particles may be accomplished at the using simpler mathematical model “hot single particle – polymeric material – air”.

Figure 2. Isotherms (T, K) at ignition moment $t_a=0.087$ s, $L=0.25$ (a), $t_a=0.092$ s, $L=0.5$ (b), $t_a=0.096$ s, $L=1$ (c) at $T_p=900$ K:
1 – gas mixture, 2 – hot steel particle, 3 – PMMA
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