Software for numerical simulation of the combustion of aluminum particles suspended in air

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Abstract. This paper presents a computer model for studying the processes of ignition and combustion of air suspended aluminum particles, based on a system of differential equations of the gas phase balance and the probability density function for temperature and particle size. The model is implemented as software for a two-dimensional non-steady state case. A new implicit difference scheme consisting in two- and three-point approximations for the first and second derivatives is proposed and implemented. A set of calculations is performed and the results of the reacting mixture characteristics distribution, the areas of the maximum heat release and their relationship with the most air suspension probable state are presented.

1. Introduction
Currently, powdered metals are used as additives to fuel in propellants to improve their energy characteristics [1,2]. One of the promising tendencies is numerical modeling [3], which allows obtaining necessary data to realize potential advantages of powdered metals (PM) without carrying out expensive full-scale experiments and use of special equipment. In this case, the description of the continuous distribution of the characteristics of the dispersed phase parameters of their physical state [4-9], in particular, temperature, size, speed is an inherent feature to focus on. For this purpose, a promising method using the probability density function (PDF) for several physical quantities is used, which allows taking into account the differences in the temperature of the gas and particles, to describe the kinetic and diffusion fuel with the oxidizing interaction, as well as to take into account the speed of the gas and particles, the effect of turbulent fluctuations on the integral and averaged values of the rates of chemical reactions and heat flows. The purpose of the work is to develop a software for the numerical simulation of aluminum particles combustion with the use of two-dimensional PDF for temperature and radius of particles.

2. Problem definition
Modeling of PM combustion, for example, aluminum, is based on the fundamental laws of energy transfer, motion, heat and mass amount and reagents mass acknowledging the presence of volumetric
The geometry of the computational domain and the general scheme of the process are shown in figure 1:

Figure 1. Geometry of the computational domain and an overview of the process

Here $x_0 = 0$ is the coordinate at the left boundary at which the particles enter the working zone (the combustion chamber) with constant initial values of particle velocity ($u_k$), gas velocity ($u$), temperature and particle radius ($r_k$ and $r$). Sliding conditions are applied on the upper ($y = y_{\text{max}}$) and lower ($y = 0$) boundary. On the right boundary ($x = x_{\infty}$), "soft" boundary conditions are applied. Initially the particles are on the left border. The particles are further heated by hot gas spreading all over the chamber. The parameters of the particles change impacted by the heat released under the chemical reaction.

The process of combustion of polydisperse aluminum particles in an air suspension is described using a PDF in which time $t$, coordinates $x$, $y$, radius $r_k$ and the temperature $T_k$ of the aluminum particles serve as arguments, $P(t, x, y, T_k, r_k)$. The product $P(t, x, y, T_k, r_k)dT_kdr_k$ is the probability that, for a particle located at the time $t$ in the coordinates $(x, y)$, the values of $r_k$, $T_k$ belong to the intervals $r_k \in (r_k, r_k + dr_k)$ and $T_k \in (T_k, T_k + dT_k)$, respectively. Using the concept and the balance equation of the PDF controlled by the normalization condition, the differential equation of the number particle concentration balance ($n_k$) can be introduced:

$$\frac{\partial n_k}{\partial t} + \int \frac{\partial n_k^0}{\partial t} P dx dy dT_k + \int \frac{\partial n_k^1}{\partial t} P dx dy dT_k - \int \frac{\partial^2 n_k}{\partial r_k^2} P dx dy dT_k = 0$$

and

$$\omega_k \frac{\partial n_k P}{\partial T_k} + \frac{\partial n_k}{\partial T_k} P \frac{\partial T_k}{\partial t} + D \left( \frac{\partial^2 n_k}{\partial x^2} P + \frac{\partial^2 n_k}{\partial x \partial y} P + \frac{\partial^2 n_k}{\partial y^2} P \right) + \frac{\partial n_k}{\partial r_k} P + \frac{\partial f_k n_k P}{\partial r_k} = 0$$

where $D$ is the particles diffusion coefficient; $\omega_k$ and $f_k$ are the particle temperature and radius rate of change(K/s and m/s), which are determined based on empirical macrokinetic data on ignition and combustion of aluminum particles [3], $n_{ok}$ is the an effective oxidant concentration, $n$ is the exponent, $T_0$ is the initial temperature in the combustion chamber:

$$f_k = \frac{dr_k}{dt} = \frac{\alpha}{n_{ok} \rho_{P1} 0.1 (T_0)^{0.2}} nr_k^{n-1},$$

$$\omega_k = \frac{dT_k}{dt} = \frac{Q}{4\pi r_k^2 \left( \frac{r_k C_2 \rho_2}{2} + \delta_1 C_1 \rho_1 \right)}.$$
(assuming a one-parameter model of turbulence and isobaric regime of the flow) in the Euler variables to describe the gas phase state, which is a mixture of several components:

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho u) = \sum_j G_j
\]

\[p=(1-z)\rho RT\]  
\[\rho C \frac{\partial T}{\partial t} + \rho u \frac{\partial T}{\partial x} = \text{div}((\lambda + \lambda_T) \text{grad} T) + Q\]  
\[\left\{ \frac{\partial m_i}{\partial t} + \rho u \text{grad} m_i \text{div}(D + D_T) \text{grad} m_i \right\} \pm G_j\]

where \( \tau \) the time, \( \rho \) is the density (kg/m\(^3\)), \( u \) - the velocity (m/s), \( p \) - the pressure (PA), \( Q \) - the source term of the heat flux in the gas phase (J/(m\(^3\)/s)), \( G_j \) - the source term formation or disappearance of the \( i \)-th gas component mass rate (kg/(m\(^3\)/s)), \( C \) - is the specific heat (J/(kg*K)), \( T \) - is the temperature (K); \( \lambda, \lambda_T \) are the molecular and turbulent thermal conductivity coefficients (W/(m*K)); \( D, D_T \) are the gas molecular and turbulent diffusion coefficients (m\(^2\)/s); \( m_i \) is the relative mass concentration of the \( i \)-th component; \( R \) is the gas constant(J/(kg*K)), \( z \) is the relative mass concentration of the \( k \)-phase components of the gas phase. The density \( \rho \), the specific heat \( C \), the molecular thermal conductivity coefficient \( \lambda \) and the molecular diffusion coefficient \( D \), are treated as functions of the gas temperature, defined as follows [3]:

\[\rho = \frac{\rho_{at}}{R_{air} T},\]
\[C = 10^{-3} + 0.87 \cdot (T - 300),\]
\[\lambda = 26.2 \cdot 10^{-3} + (T - 300) \cdot 7.6 \cdot 10^{-5},\]
\[D = 0.178 \cdot 10^{-4} - \frac{4 \cdot T}{273},\]

where \( \rho_{at} \) - atmospheric pressure, \( R_{air} \) - universal gas constant for air.

The source terms \( G_j \) and \( Q \) are determined taking into account the convective and radiative heat transfer mechanisms and assuming a one-step chemical reaction

\[\text{Al} + \frac{3}{4} \text{O}_2 \rightarrow \frac{1}{2} \text{Al}_2\text{O}_3 + \Delta H\]

using the PDF [3]:

\[Q = \Delta H \int \int 4\pi r_k^2 \rho_k n_k f_k P dT_k d\tau_k - \int \int 4\pi r_k^2 \rho C \rho_k n_k \omega_k f_k P dT_k d\tau_k,\]

\[G = K_{m0} \int \int 4\pi r_k^2 \rho_k n_k f_k P dT_k d\tau_k,\]

where \( K_{m0} \) is the mass stoichiometric coefficient.

The initial values of the parameters in the combustion chamber at \( \tau = 0 \) (these parameters are denoted by the index 0): pressure \( p = 0.1 \text{ MPa} \), temperature \( T_0 = 300 \text{ K} \), gas velocity \( u_0 = 1 \text{ m/s} \), relative mass concentrations \( m_{02} = 0.23, m_{Al} = 0.77 \). This work features powdered aluminum in the function of fuel with the lognormal radius distribution of the particles number. The particles are ignited by a hot gas, which is filled in space \( x_0 < x < x_\infty \) and has a constant temperature \( T_{ig} = 2300 \text{ K} \) (the particles reach this temperature at the flame front).

3. Difference scheme

3.1. Difference approximation

Differential equations (1)-(5) are approximated by first-order time-precision and first-order space-accuracy difference equations. For this purpose, a uniform grid is introduced along the coordinate axes \( \text{OX} (0 \leq i < N) \), \( \text{OY} (0 \leq j < M) \), the time axis \( \text{or, and the axes of the particle parameters} \), \( \text{o}\tau_k \) \( (0 \leq q < q_{max}) \) and \( \text{o}\tau_k \) \( (0 \leq s < s_{max}) \). As a result, we pass to the equations of run (7)-(11):
\[
\begin{align*}
A_x v_{i-1,j} + B_x v_{i,j} + C_x &= 0 \\
A_y w_{i-1,j} + B_y w_{i,j} + C_x &= 0 \\
A_T T_{i-1,j} + B_T T_{i,j} + C_T T_{i,j} + D_T T_{i,j+1} + E_T T_{i,j+1} &= -F_T \\
A_m m_{i-1,j} + B_m m_{i,j} + C_m m_{i,j} + D_m m_{i,j+1} + E_m m_{i,j+1} &= -F_m \\
A_n n_{i,j} + B_n n_{i-1,j} + C_n n_{i,j} + D_n n_{i,j+1} + E_n n_{i,j+1} + F_n n_{i,j+1} &= -G_n \\
A_p P_{i,j} + B_p P_{i,j} + C_p P_{i,j} + D_p P_{i,j+1} + E_p P_{i,j+1} + F_p P_{i,j+1} + G_p P_{i,j+1} + H_p P_{i,j+1} &= I_p
\end{align*}
\]

where \( v \) is the projection of the gas velocity on the OX axis, \( w \) is the projection of the gas velocity on the OY axis.

Each equation (8)-(10) is written as a row in a five-diagonal matrix, and the index in the coefficient column is calculated by the following formula: if the coefficient \( K \) belongs to the variable \( T_{i,j} \), then its index in the row is equal to \( index = i \cdot M + j \). Initially, no more than 6-7 elements (less than 1%) are entered in each row of the matrix. However, as a result of intermediate calculations, a number of the zero coefficients will turn into non-zero ones.

Equation (11) is written as a string in eight-diagonal matrix, and the index in the column of the coefficient is calculated according to the following formula: if the \( K \)-factor refers to a variable \( P_{i,j}^{qs} \), then its index in the string is equal to \( index = i \cdot M \cdot q_{max} \cdot s_{max} + j \cdot q_{max} \cdot s_{max} + q \cdot s_{max} + s \). Initially, each row of the matrix features not more than 9 items (less than 1%). However, as a result of intermediate calculations, a number of the zero coefficients will turn into non-zero ones.

In each equation, the maximum coefficient is at the central node of the scheme \((B_x, B_y, C_T, C_m, C_n, C_p)\), thus, on the principle of maximum\([12-14]\), the proposed implicit difference scheme is stable.

### 3.2 Algorithm for solving the problem

To reduce the time of calculations, the calculations are narrowed (stored and performed) to the ones with non-zero coefficients, allowing to reduce the size of the matrix by N/3 times.

To improve the accuracy of calculations, the values of temperature, particle radius, relative mass of the gas suspension component and spatial coordinates are transformed into a dimensionless form as follows:

\[
\begin{align*}
\theta_T &= \frac{T_k - T_k^0}{T_{max} - T_k^0} , \\
\theta_r &= \frac{r_k - r_k^{min}}{r_k^{max} - r_k^{min}} , \\
\theta_x &= \frac{x - x_0}{x_{\infty} - x_0} , \\
\theta_y &= \frac{y - y_0}{y_{\max} - y_0} ,
\end{align*}
\]

where \( r_k^{min} = 0.5 \ \mu m, r_k^{max} = 6 \ \mu m, T_k^{max} = 2300 \ \text{K}, x_0 = 0 \ \text{cm}, x_{\infty} = 5 \ \text{cm}, y_0 = 0 \ \text{cm}, y_{\max} = 3 \ \text{cm} \).

The matrices of the running coefficients from the equations (7)-(11) are sparse, so the Gauss method for calculating only non-zero elements was modified to accelerate the calculations. An open-source database Redis key-value database is used to store items. As operations of writing/reading to/from the database take a long time, the software uses the buffered input/output. To visualize the results of calculations QtDataVisualization library, consisting of classes Q3DSurface, QSSurfaceDataProxy, QHeightMapSurfaceDataProxy, QSSurface3DSeries is used.
3.3 Features of the computing

The algorithm of calculations (figure 2) finishes working upon meeting one of two conditions: either the flame front (the zone of the greatest density of heat release) has stabilized, or the maximum number of iterations is exceeded (in this work the maximum number of iterations was 25). The combustion process may not stabilize if velocities of the particles when they enter the combustion camera are too high or too low: the flame front may move beyond the boundaries of the computational domain or to fluctuate around the coordinates x=0.

A new implicit difference scheme featuring a three-point template for calculating the gas velocity, five-point templates for calculating the gas temperature and relative mass concentrations, a six-point template for calculating the particle concentration and an eight-point template for calculating the values of the PDF is proposed and implemented. All first derivatives are approximated by left-sided difference derivatives, and all second derivatives are approximated by central difference derivatives.

![Figure 2. The scheme of algorithm calculation software](image)

4. Calculation results

Figure 3 shows the temperature distribution graph of the particles in the combustion chamber. As the
particles pass from the wall $\theta_x=0$ to the wall $\theta_x=1$ the temperature of the particles reaches its maximum (combustion temperature) and the hot particles are located either on the axis $\theta_y=0.5$ in the center of the combustion chamber, or along the borders (walls) $\theta_y=0$ and $\theta_y=1$.

Figure 3. Temperature distribution of particles in the combustion chamber

Figure 4 shows the gas velocity distribution in the combustion chamber, indicating that the gas moves from the wall $\theta_x=0$ to the wall $\theta_x=1$, the speed increases sharply and the highest speed is observed either on the axis $\theta_y=0.5$ in the center of the combustion chamber, or near the walls $\theta_y=0$ and $\theta_y=1$.

Figure 4. Velocity distribution of particles in the combustion chamber

Figure 5 shows a two-dimensional PDF in the flame front. This graph is characterized by the presence of two local maxima corresponding to the state of the particles close to the initial state and combustion in the vapor mode, the number of the latter is $\sim 25\%$. 
The modelling results were compared with the experimental data on the propagation of the flame through the aluminum air suspension in the model combustion chamber presented in [3] in order to verify the numerical model. A satisfactory qualitative agreement on the gradient of temperature change and heat release in the combustion chamber is obtained with the difference between the calculated and experimental gradients of the temperature change values not exceeding 9.7%.

5. Conclusions
1. A mathematical model of the processes of ignition and combustion of aluminum particles air suspension using the function of the density distribution of the probability of temperature and particle size in a non-stationary two-dimensional space setting, a numerical method and an algorithm for solving a system of differential equations describing the state of the dispersed and gas phases were developed.

2. The created algorithm for solving the problem is implemented in a software with a user interface that allows swiftly changing the initial conditions of the calculation in order to study the effect of the main parameters of the gas suspension and the geometric characteristics of the combustion chamber on the macrokinetic and integral characteristics of the ignition and combustion.

3. The features of the processes of ignition and combustion of aluminum-air mixture and obtained data on the likelihood of their condition in different zones of the combustion chamber were analyzed using the created software.

References
[1] Milehin Yu M, Klyuchnikov A N, Burskii G V 2013 Energetika raketnih dvigateley na tverdom toplive (Moscow: Nauka) p 207
[2] Davis A 1963 Solid Propellants. The Combustion of particles of metal ingredients Combustion and flame 7-4 pp 359-367
[3] Yagodnikov D A 2009 Ignition and combustion of powdered metals (Moscow) p 432
[4] Yagodnikov D A 1996 Statistical model of flame front propagation in a boron-air mixture Combustion, explosion and shock waves 32-6 pp 29-46
[5] Yagodnikov D A, Gusachenko E I 2002 Effect of an external electric field on the disperse composition of condensed products of aluminum particle combustion in air Combustion, Explosion and Shock Waves 38-4 pp 449-455
[6] Chena Yi, Guildenbechera D R, Hoffmeistera K N G, Copera M A, Stauffachera H L, Olivera M S, Washburnb E B 2017 Study of aluminum particle combustion in solid propellant plumes using digital in-line holography and imaging pyrometry Combustion and Flame 182
pp 225-237

[7] Vilyunov V N, Vorozhtsov A B, Feshchenko Yu V 1989 Modeling of two-phase flow of a gas mixture with burning metal particles in a semi-enclosed duct Combustion, explosion and shock waves 25-3 pp 39-43

[8] Basevich V Ya, Volodin V P, Peregudov N I 1990 Determining the probability density function of the temperature by calculating a turbulent flame from the instantaneous parameters // Combustion, explosion and shock waves 26-6 pp 22-26

[9] Yagodnikov D A, Voronetsky A V 1992 Effect of velocity nonequilibrium on the laminar flame propagation characteristics in an air-dispersed medium Combustion, explosion and shock waves 28-5 pp 38-44

[10] Shchetinin G A 2017 Numerical simulation of aluminum particle aerosol combustion employing a probability density function Politechnical student journal of BMSTU (Moscow)

[11] Gavin L V, Medvedev V A, Naumov V A 1988 Model of a two-phase turbulent jet with heterogeneous particle combustion taken into account Combustion, explosion and shock waves 24-3 pp 12-17

[12] Samarskii A A, Popov Yu V 1975 Difference schemes of gas dynamics (Moscow: Nauka) p 109.

[13] Shian A F, Shian N B 2015 Optimization of educational computational experiment based on the use of online services in solving differential equations Modern problems of science and education (Penza: Publishing House "Academy Of Natural Sciences") 1 pp 10-12

[14] Saidakhmat K E 2015 The decision of a problem of nonlinear optimization of thermal processes described by the Volterra integro-differential equations News of Academy of Sciences of the Republic of Tajikistan. Department of physical, mathematical, chemical, geological and technical sciences 3 (Dushanbe: Presidium of the Academy of Sciences of the Republic of Tajikistan) pp 31-38