Ignition and combustion of polydispersed dust in turbulized flows.

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Keywords: multiphase flow, polydispersed, dust, turbulence, combustion, devolatilization, flame zone, ignition limits, size-distribution, nonuniformity.

Abstract.

The mathematical model for turbulent combustion and ignition of polydispersed dust-air mixtures is developed. The worked out mathematical model takes into account the two-way coupling effects in gas-particles interactions and combines both deterministic and stochastic approaches. The equations of motion for particles take into consideration the influence of random turbulent pulsations in the gas flow. The models for phase transitions and chemical reactions take into account thermal destruction of dust particles, vent of volatiles, chemical reactions in the gas phase and heterogeneous oxidation of carbon by O_2 and CO_2 influenced by both diffusive and kinetic characteristics.

The system of equations for gas phase was obtained by Favre averaging the system of multicomponent multiphase media [1].

Averaging by Favre with the $\alpha\rho$ weight [2, 3] we obtain the following system for the gas phase in a multiphase flow [4] (the averaging bars are removed for simplicity):

$$\partial_t(\alpha\rho) + \nabla\cdot(\alpha\rho\vec{u}) = \dot{M} \quad (1)$$

$$\partial_t(\alpha\rho Y_k) + \nabla\cdot(\alpha\rho\vec{u}Y_k) = -\nabla\cdot\vec{I}_k + \dot{M}_k + \dot{\omega}_k \quad (2)$$

$$\partial_t(\alpha\rho\vec{u}) + \nabla\cdot(\alpha\rho\vec{u}\otimes\vec{u}) = \alpha\rho\vec{g} - \alpha\nabla p + \nabla\cdot\tau + \dot{\vec{K}} \quad (3)$$

$$\partial_t(\alpha\rho E) + \nabla\cdot(\alpha\rho\vec{u}E) = \alpha\rho\vec{u}\cdot\vec{g} - \nabla\cdot p\vec{u} - \nabla\cdot\vec{I}_q + \nabla\cdot(\tau\cdot\vec{u}) + \dot{E} \quad (4)$$

The equations (1-4) include mass balance in the gas phase, mass balance of k-th component, momentum balance and energy balance respectively. We have the following relationships between the terms in the equations (1-2):

$$\sum_k Y_k = 1\ ,\quad \sum_k \dot{M}_k = \dot{M}\ ,\quad \sum_k \vec{I}_k = 0\ ,\quad \sum_k \dot{\omega}_k = 0\ .$$

The state equations for gaseous mixture are the following:

$$p = R_g\rho T\sum_k Y_k W_k^{-1}\ ,\quad E = \sum_k Y_k(c_{vk}T + h_{0k}) + \frac{\vec{u}^2}{2} + k\ . \quad (5)$$

Two chemical reactions in the gas phase were considered: generalized volatiles component L oxidizing (unidirectional) and carbon monoxide CO oxidizing (reversible). The k-th component mass origination rate $\dot{\omega}_k$ was calculated using the Arrønius law for the reactions' rate; averaged magnitudes for mass fractions, temperature and density were used in the law as the first approximation.

The turbulent heat flux $\vec{I}_q$ in the equation (4) is a sum of two terms:

$$\vec{I}_q = \vec{J}_q + \sum_k (c_{pk}T + h_{0k})\vec{I}_k\ , \quad (6)$$

where $\vec{J}_q$ could be interpreted as turbulent conductive heat flux.

The eddy kinematic viscosity ν^t is expressed according to k-epsilon model as $\nu^t = C_\mu k^2/\varepsilon$.

Using the standard k-epsilon model for compressible flows [3], we will model the turbulent fluxes in the following way:

$$\tau = \alpha(\mu + \rho\nu^t)(\nabla\vec{u} + \nabla\vec{u}^T - (2/3)(\nabla\cdot\vec{u})U) - (2/3)\alpha\rho kU\ , \quad (7)$$

$$\vec{I}_k = -\alpha\rho(D + (\nu^t/\sigma_d))\nabla\cdot Y_k\ , \quad (8)$$

$$\vec{J}_q = -\alpha(\lambda + \sum_k c_{pk}\rho(\nu^t / \sigma_t))\nabla \cdot T, \qquad (9)$$

The model is closed then by 2 equations for k and ε:

$$\partial_t(\alpha\rho k) + \nabla\cdot(\alpha\rho\vec{u}k) = \nabla\cdot(\alpha(\mu + \rho(\nu^t/\sigma_k))\nabla k) + \tau^t : \nabla\vec{u} - \alpha\rho\varepsilon\ , \qquad (10)$$

$$\partial_t(\alpha\rho\varepsilon) + \nabla\cdot(\alpha\rho\vec{u}\varepsilon) = \nabla\cdot(\alpha(\mu + \rho(\nu^t/\sigma_\varepsilon))\nabla\varepsilon) + (\varepsilon/k)(C_{1\varepsilon}\tau^t : \nabla\vec{u} - C_{2\varepsilon}\alpha\rho\varepsilon)\ , \qquad (11)$$

The constants take the following standard values [5, 13]:

$$C_\mu = 0.09,\quad C_{1\varepsilon} = 1.45,\quad C_{2\varepsilon} = 1.92,\quad \sigma_d = 1,\quad \sigma_t = 0.9,\quad \sigma_k = 1,\quad \sigma_\varepsilon = 1.13. \qquad (12)$$

With the equations (10-11) and expressions (7-9) in order to close the model one needs to define expressions for mass, momentum and energy fluxes from the other phases ($\dot{M}, \dot{M}_k, \dot{\vec{K}}, \dot{E}$).

The motion of polydispersed particulate phase is modeled making use of a stochastic approach. A group of representative model particles is distinguished. Motion of these particles is simulated directly taking into account the influence of the mean stream of gas and pulsations of parameters in gas phase:

$$m_i\frac{d\vec{v}_i}{dt} = m_i\vec{g} - \frac{m_i}{\rho}\nabla p + \vec{f}_d\ , \qquad \frac{d\vec{r}_i}{dt} = \vec{v}_i \qquad (13)$$

where the force affecting the particle consists of gravity and Archimedus forces, resistant force and Langevin force. The Langevin force which models turbulent pulsations is evaluated together with the resistance force using the random vector $\vec{w}_i$ determined independently for each model particle:

$$\vec{f}_{di} = \frac{1}{2}C_d(\mathbf{Re}_i)\rho S_i(\vec{u} + \vec{w} - \vec{v}_i)|\vec{u} + \vec{w} - \vec{v}_i|\ , \qquad (14)$$

The model was validated in comparison with experiments on organic dust combustion in confined volumes under different levels of initial turbulization of mixture. The validation was based on a set of experiments on ignition and combustion of dextrin-air mixtures [5] carried out in a cylindrical 1.25 m^3 vessel.

The mean flame trajectories being a result of averaging are shown in the fig. 1 for a low initial level of turbulence (RMS= 1.4 m/s). The right axis of the fig. 1 reflects the pressure increase inside the vessel detected by a pressure gauge located on the wall. Arrows on the curves point the axis relating to the curve. Circles of different shade reflect the dynamics of flame forefront position for different directions from the center and different experiments. Those results reflect irregularity of the flame zone behavior. The solid curve presents the averaged trajectory of flame front expansion from the center.

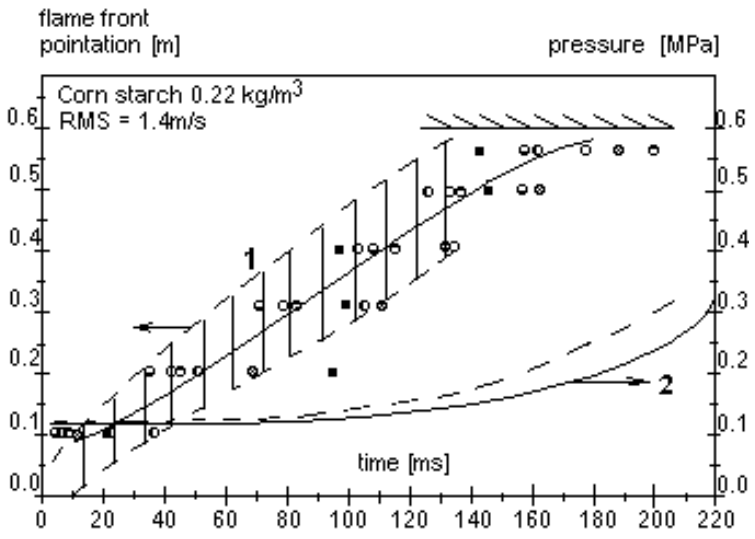

fig. 1

Dashed zone in the fig. 1 presents the results of the numerical modeling of turbulent flame propagation for the same value of initial turbulence. The flame boundaries were detected along five central rays (in horizontal, vertical directions and 45 degrees to the horizon) as points of maximal gradients of volatiles oxidizing intensity function on the each ray. The dashed zone in the fig. 1 presents the flame trace being the result of averaging in those five directions. The dashed curves 1 bounding the dashed zone were obtained by estimating the position of the forefront and the rear front of the flame. The dashed curves 2 in the fig. 1 show the growth of the mean wall pressure obtained as a result of averaging (the ratio of integral of pressure to to the wall surface area). Comparison shows a satisfactory coincidence of numerical and experimental data.

Mathematical models provide a powerful tool to investigate the sensitivity of polydispersed mixtures ignition and combustion characteristics to variations of governing parameters, because it is only in numerical experiments that the influence of each factor could be studied independently and the rest of conditions could be maintained constant for all the experiments. The opportunity that could hardly be provided by physical experiments.

The developed mathematical model made it possible to investigate the peculiarities of polydispersed organic dusts ignition and combustion and the influence of flow nonuniformities on the ignition limits.

A series of numerical simulations for the dust particles – oxygen mixtures was performed. The variable parameter was the average density of the particulate phase ρ_{av}. The mean flame trajectory was determined as the evolution of the maximal gradient of the oxygen concentration using the averaging in five directions described above.

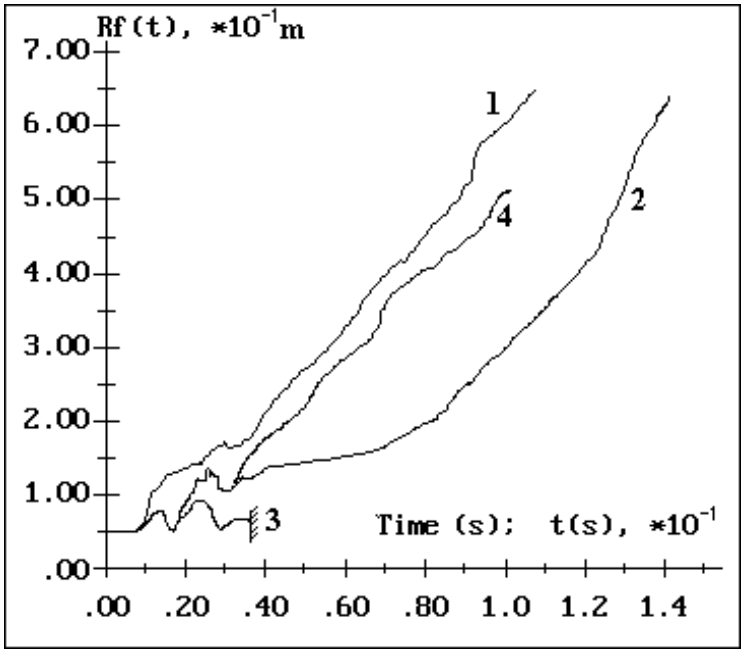

fig. 2

The fig. 2 shows the flame trajectories for the cases of different concentration of the particulate phase: curve 1 – ρ_{av} = 0.25 kg/m^3, curve 2 – ρ_{av} = 0.22 kg/m^3, curves 3, 4 – ρ_{av} = 0.20 kg/m^3. The ignition energy and characteristic time were considered: $E_0 = 1.55 \cdot 10^3$ J, $t_0 = 10^{-2}$ s. The curve 1 (fig. 2) reflects the case when self-sustaining combustion starts just after switching off the ignitor but then the flame propagation starts. The curve 3 corresponds with the "no-ignition" case: the combustion of particles within the ignition zone continues for some time after switching off the ignitor and then the combustion extinguishes. Thus the mixture ρ_{av} = 0.20 kg/m^3 is below the ignition limit under the given ignition conditions.

Let us regard the influence of non-uniformity of dust concentration distribution on the ignition. We consider the same average dust content ρ_{av} = 0.20 kg/m^3 but linearly distributed in the vertical direction so that the dust content at the top ρ_{min} = 0 kg/m^3; at the bottom ρ_{max} = 0.4 kg/m^3 and in the center ρ_{med} = 0.2 kg/m^3 (the same as in the previous experiment). This type of particles concentration distribution is very common for the sedimenting dust clouds.

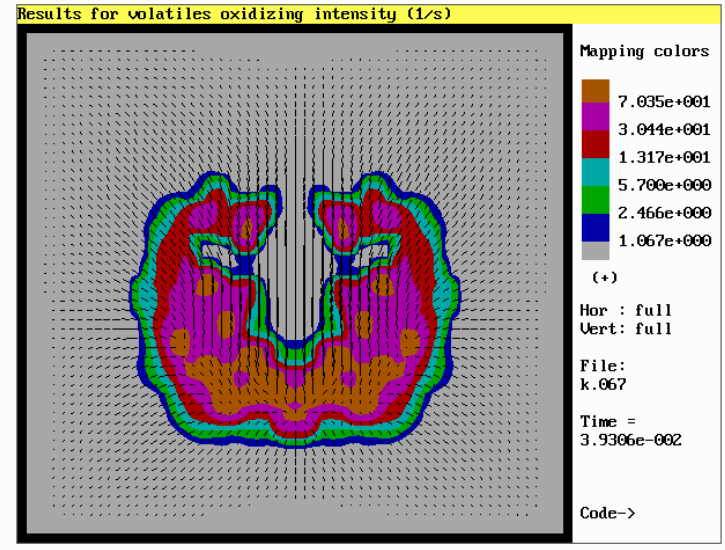

fig. 3

The results of numerical modeling show that under the nonuniform dust distribution the ignition does take place contrary to the uniform distribution. The flame trajectory for the case of nonuniform dust concentrations is shown in the fig. 2 (curve 4). After switching off the ignitor the scenario of the "slow ignition" takes place and in some time a self-sustaining flame zone is formed. The zone propagation is not symmetrical: it propagates more rapidly in the lower part of the vessel where the dust concentration increases. But then after the strong turbulent combustion zone is formed it propagates also in the upward direction. A characteristic map of the reaction zone is shown in the fig. 3. The nonsymmetrical flamezone propagation (fig. 3) brings to a strong flow of hot reaction products from the lower into the upper part of the vessel that causes the forced convective ignition of the upper less dense mixture layers. Thus the nonuniformity of the particulate phase distribution in the

polydispersed mixtures creates more favorable conditions for the ignition. The numerical results could be summarized as follows.

The combustion zone in heterogeneous mixtures is shown to be very wide having an irregular structure with a number of hot spots. Its propagation velocity strongly depends on initial turbulence, particles size distribution, concentration of oxygen in gas. The increase of particles size and oxygen concentration brings to the increase of the reaction zone width and irregularity. The increase of the initial level of turbulence promotes the flame propagation but inhibits ignition near the limits. The decrease of the mean dust volumetric concentration lowers down the flame propagation velocity and creates less favorable ignition conditions near the limits. The nonuniformity of the particulate phase distribution in the mixture creates more favorable conditions for ignition and lowers the ignition limits. These preliminary results show the necessity of more detailed investigations of ignition limits for polydispersed mixtures with inhomogeneous distribution of condensed phase typical for the majority of practical cases.

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