Simulation of Detonation in Particulate Systems with Applications to Pulse Detonation Engines

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Abstract
Reacting two-phase flows attract particular interest because of their applicability to pulse detonation engines. Use of laser pulse allows to create desired temporal and spatial distributions of ignition centres and to perform a homogeneous ignition within the sub-microsecond interval. The injection of metal particles with low evaporation temperature and ionization potential or liquid droplets causes optical breakdown on individual particle or droplet, and leads to drop of detonation minimum pulse energy of the mixture. The physical and mathematical models and up-to-date numerical methodology for computer modelling are developed and validated. Laser-induced detonation in particulate systems is studied, and possibilities of the new methodology are demonstrated.

Introduction

A pulse detonation engine is an unsteady propulsive device in which the combustion chamber is periodically filled with a reactive gas mixture, a detonation is initiated, the detonation propagates through the chamber, and the product gases are exhausted. The high pressures and resultant momentum flux out of the chamber generate thrust. Use of laser pulse allows to create desired temporal and spatial distributions of ignition centres and to perform a homogeneous ignition within the sub-microsecond interval.

The reactive metal particles are used to enhance blast performance. Although the total energy released by the metal combustion is significant and comparable to the total energy released by the explosive itself, the timescale of this energy release (timescale of particle reaction) for typical particle sizes (from 1 to 100 μm), is too long to contribute directly to the detonation front itself. The metal particles react with gas or detonation products behind the blast wave. It has been shown that the metal particle reaction significantly increases the strength of the blast and the total impulse delivered to nearby objects or structures [1].

Processes that control transport and combustion of particles and droplets remain unresolved, and introduce significant uncertainties into modeling and simulation. One of the most important parameters for practical applications is the minimum pulse energy (MPE) required to induce ignition and detonation of the mixture.

When a power laser pulse ($I_* \sim 10^{11}$ W/cm^2) interacts with a gas, the gas breaks down and becomes highly ionized [2, 3]. This process is always accompanied by a light flash and generation of sound. The development of electron cascade requires the existence of initial free electrons in a gas.

Particles or droplets, trapped by a laser beam, considerably influence results of the process [4]. It is well known from experiments that for every particle size of any material there is threshold intensity at which the particle material converts into the meta-stable condition and its intense evaporation leads to heat destruction of the particle, either by means of local jetting of the essential part of the particle mass or due to explosion of the particle (optical breakdown).

The injection of metal particles with low evaporation temperature and low ionization potential (e.g., aluminium) leads to drop of detonation MPE ($I \sim 10^9$ W/cm^2) due to optical breakdown on individual particles. Vapour aureole around metal particle is a source of free electrons, and optical breakdown in the gas-particle mixture comes for lower energy of laser pulse than in pure gas.

Many experimental, theoretical and numerical studies have been performed for the past years [4–10]. However, some fundamental and practical problems are yet to be resolved. They include qualitative and quantitative description of processes around individual particle and droplet, knowledge in particle microphysics and optical properties of particles, sub-models of heating and evaporation, transport of aggregates of complex morphology, threshold values of optical breakdown, dependence of MPE on the contributing factors (laser pulse, composition of gas mixture, shape of particles).

The classical Chapman–Jouguet (CJ) theory is not applicable to the modelling of the detonation of gas-particle mixtures because the time of particle burning is by one or more orders of magnitude longer than that of reaction between gaseous species. The detonation velocities are up to 20–40% less than those predicted by the equilibrium CJ theory [11]. The coupling between the shock front and the reaction zone is modified by addition of particles due to chemical reactions between particles and gas. The momentum and heat transfer are responsible for the velocity deficit with respect to detonation in pure gas.

The detonation wave structure and detonation stability in mixtures of reactive gases and solid particles was studied in [5] for 1D and 2D flows. Increasing the parti-

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cle volume fraction results in a rapid drop of the detonation wave speed, and smaller particle diameters resulted in slightly lower detonation velocities. A detonation suppression in a stoichiometric hydrogen–oxygen mixture by means of injection of chemically inert particles was simulated in [12].

Ignition and reaction of metal particles in a high explosive environment was studied in [13]. The ignition delay time observed in experiments and computational analysis was a result of convective heating of the particle to a critical temperature for chemical reaction.

Physical and mathematical models of optical breakdown on individual particle and droplet, and up-to-date numerical methodology for computer modeling are developed. Laser-induced detonation in gas-particle and gas-droplet mixtures is studied, and advantages of the new methodology are demonstrated. The in-house computer code has been developed, and contribution of parameters of laser pulse and composition of the mixture is studied. Comparison of some numerical results with experimental data is made.

Laser pulse

The time of laser pulse, its shape and intensity define the interaction of laser pulse with individual particle or droplet and mixture.

The intensity of laser pulse is represented as a product of the maximal intensity, I_0, the function describing the time distribution of the intensity, $f_1(t)$, the function taking into account the spatial distribution of the intensity, $f_2(r)$, and the function describing absorption of radiation in the medium, $f_3(z)$. The intensity of laser pulse is

$$I(t, r, z) = I_0 f_1(t) f_2(r) f_3(z),$$

where t is time, r is radial coordinate, and z is coordinate indicating direction of propagation of laser beam.

The theoretical peak intensity of laser pulse at any radial point is calculated for given power and degree of focus. The laser does not reach its peak operating power at the moment when it is turned on. It requires a short time to ramp up to its peak output. For a laser pulse which lasts 8 μs, the laser output reaches its peak intensity in about one fourth of a pulse duration and will have dropped to roughly three fourth of its peak value when the laser is shut off. The laser model includes a ramp time parameter during which time the laser's output increases linearly to a maximum (Figure 1).

The time distribution of the intensity is represented by a continuous piecewise-linear function

$$f_1(t) = \sum_{k=1}^{N-1} \left[I_k + (I_{k+1} - I_k) \frac{t - t_k}{t_{k+1} - t_k} \right] \phi(t_k, t_{k+1}),$$

where t_k and I_k are time and intensity of laser pulse, and N is a number of ramp points. The function $\phi(t_k, t_{k+1})$ is given by

$$\phi(t_k, t_{k+1}) = \frac{t - t_k + |t - t_k|}{2|t - t_k| + \varepsilon} - \frac{t - t_{k+1} + |t - t_{k+1}|}{2|t - t_k| + \varepsilon},$$

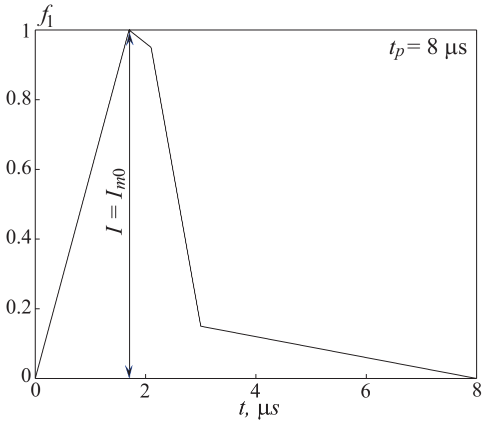

Figure 1. Intensity of laser pulse as a function of time.

where ε is the small value used to avoid division by zero.

A continuous piecewise-linear representation of pulse shape is used to compute the temporal characteristic

$$S = \int_0^\infty f_1(t) dt = \frac{1}{2} \sum_{k=1}^{N-1} \frac{I_{k+1} + I_k}{t_{k+1} - t_k}.$$

In a plane normal to the direction of laser pulse, the spatial distribution of the intensity is described by the normal distribution (Figure 2)

$$f_2(r) = \exp\left(-\frac{2r^2}{R^2}\right),$$

where r is a radial distance from centreline of the laser beam, and R is a radius of laser spot.

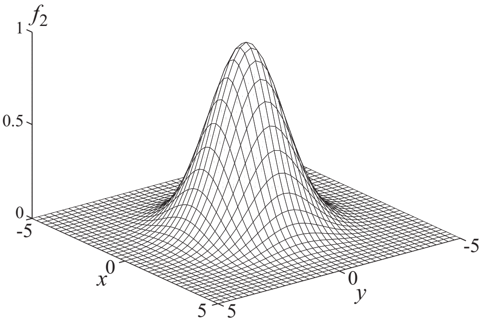

Figure 2. Intensity of laser pulse as a function of radial coordinate (radius of laser spot is 5 mm).

The absorption of radiation is described by Bouguer–Lambert–Beer law

$$f_3(z) = \exp(-\mu z),$$

where μ is the absorption coefficient depending on the nature, state and fraction of particles as well as on the wave length of laser radiation.

The total energy of laser pulse is related to its intensity

$$Q = \int_0^\infty \int_0^{2\pi} \int_0^\infty I_0 f_1(t) f_2(r) r dr\, d\varphi\, dt,$$

where φ is a polar angle.

Breakdown mechanism

Physical model of optical breakdown provides qualitative description of the processes, in particularly interaction of laser pulse with individual metal particle and liquid droplet.

Metal particle. A chain of processes leading to explosion and optical breakdown of individual metal particle was developed (Figure 3). These processes depend on optical properties of particle, its shape and ratio of particle size to radius of laser spot.

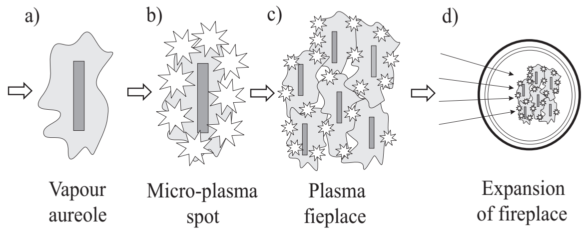

Figure 3. Optical breakdown on metal particle.

The particle is heated up to high temperature, melting and evaporation start (Figure 3a). Evaporation of a particle leads to the formation of a vapour aureole around the particle. Free electrons are generated in the vapour aureole as a result of thermal emission from particle surface (if $T < T_b$) and isothermal ionization in vapour aureole (if $T > T_b$). This leads to collisions of electrons with ions and atoms and electron–electron collisions. Ionization of vapour aureole due to reverse drag effect leads to development of electron avalanche and formation of micro-plasma spots around the particle (Figure 3b). The cascade ionization process is significant at high pressure and longer laser pulse because under these conditions, electron–atom or electron–ion collisions have sufficient time to occur during the laser pulse [3]. Micro-plasma spots are expanded due to thermal diffusion of electrons and ionisation of molecules and atoms of surrounding gas. Micro-plasma spots are merged, and plasma fireplace is formed around the ensemble of particles (Figure 3c). The plasma fireplace absorbs laser radiation, and contributes to development and propagation of self-sustaining shock wave in the gas-particle mixture (Figure 3d).

Liquid droplet. Compared to metal particle, heating and evaporation of liquid droplet are delayed due to weak absorption of laser radiation. Concentration of free electrons in vapour aureole is insufficient for development of electron avalanche. In this case, the key mechanism of development of optical breakdown is explosive evaporation of droplet (Figure 4).

The laser radiation focuses inside a droplet near its shadow side (Figure 4a). In this region, overheating conditions arise, and liquid is in meta-stable state in which its temperature exceeds the temperature of saturated vapour at given temperature. Internal vapour cavity is formed, and liquid boils off in this cavity (Figure 4b). Increase

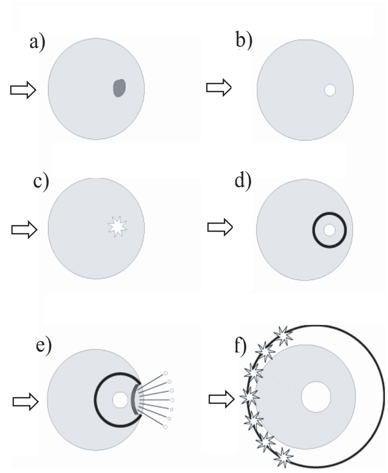

Figure 4. Optical breakdown on liquid droplet.

in pressure in the vapour cavity creates conditions for internal micro-breakdown. Internal micro-plasma spot is appeared and absorbs laser radiation (Figure 4c). Further increase in pressure in the vapour cavity forms shock wave expanding inside droplet (Figure 4d). Expansion of shock wave induces thermal ionization of surrounding gas on shock wave front (Figure 4e). Free electrons that have appeared on shock wave front induce chain mechanism of breakdown, receiving their energy due to reverse drag effect (Figure 4f). Intense vaporization of droplet leads to the thermal destruction of the droplet either by means of local jetting of essential part of droplet mass or by its explosion.

Mathematical model

The mathematical formulation of the problem is divided into low-level and high-level models. Low-level models correspond to the processes in the volume occupied by an individual particle or droplet. The high-level models correspond to the processes in the volume occupied by multi-phase mixture.

Low-level models. Low-level models describe melting, heating, evaporation and formation of vapour aureole, appearance of free electrons due to thermal ionisation on front of shock wave, and development of electron avalanche due to reverse drag effect.

To compute optical properties of particle (e.g., absorption efficiency of laser radiation), semi-empirical data are used. There are detailed data about temperature dependencies of optical, thermal and physical properties of aluminium, because it often occurs in practice.

Heating model is based on numerical solution of unsteady heat diffusive equation [8, 14].

The equations describing electron avalanche in the vapor aureole include the equation of heating of vapor aureole due to electron–atom collisions, the equation of warming-up of electrons, the ionization kinetic equation of vapor as a result of electron impact, and the equation of particle mass.

The plasma in vapor aureole is considered as an ideal gas. The Euler equations are used for the simulation of gas dynamical processes in vapor aureole.

The detailed chemistry model is not important to develop the low-level model. Use of detailed chemistry model in the volume occupied by an individual particle requires high computational costs. A simple model of one-step chemical reaction is used in order to reproduce explosion of individual particle.

Threshold value of optical breakdown on an individual particle is computed as a result of the solution of low-level models. Low-level models are incorporated in high-level models that describe detonation of the mixture.

High-level models. The multi-phase mixture consists of some gas and particulate components (Figure 5). Gas phase consists of a combustible component (fuel), an oxidant component, a component that is combustion product, and a neutral component. Particulate phase represents ensemble of metal particles and liquid droplets. Vapour phase is a product of thermal decomposition of metal particles, and it consists of atoms, ions and electrons. Condensed phase represents metal oxide that is a result of vapour condensation.

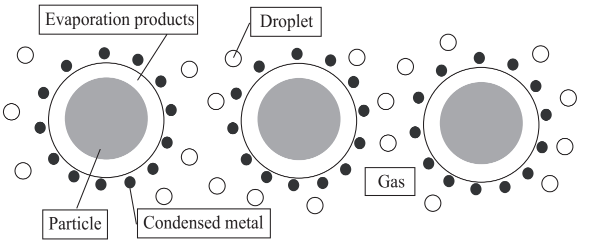

Figure 5. Composition of multi-phase mixture.

The Eulerian approach is used to formulate governing equations describing detonation of the mixture. The governing equations are written for all gas and particulate components of the mixture. The diffusion processes are ignored because they define the evolution of the mixture on the time scales, which are much longer than the time of laser pulse.

Coupling procedure. The data obtained from solution of low-level problems are used to calculate source terms in the governing equations describing high-level problem. It is assumed that particles are uniformly distributed in the domain. Some volume of the mixture depending on particle volume fraction is associated with each particle (individual reactor of a particle). The model of unsteady well-stirred reactor is used to calculate physical quantities in this volume.

Computational procedure

The problem considered is multi-physical and multi-scale. The main feature of the problem is correlation and interference of physical, gas dynamics and chemical processes, and a wide range of temporal and spatial scales. Metal particles have a non-spherical shape.

The in-house computer code has been developed. The equations are solved numerically based on finite volume method, splitting scheme on physical factors, piecewise parabolic method and Chakravarthy–Osher scheme for inviscid fluxes. Approximate Riemann solver is employed to calculate the interfacial fluxes on the first fractional time step. Chemical reactions and interphase exchange of mass, momentum and energy are considered at the second fractional time step. The internal time step is used to ensure stability of numerical scheme. Pseudo-gas of particles does not have internal pressure, so artificial pressure is introduced to design similar computational procedures for gas and particulate components.

Results and discussion

The results concern processes near individual particle and droplet, and detonation of multi-phase mixture. Particle location relative to centreline of laser beam, energy, time and shape of laser pulse vary in calculations. The output quantities are threshold value of optical breakdown and detonation MPE.

Metal particle. The Figure 6 shows heating of metal particle up to the boiling temperature. The particle temperature depends on total energy of laser pulse and distance from particle to centreline of laser beam.

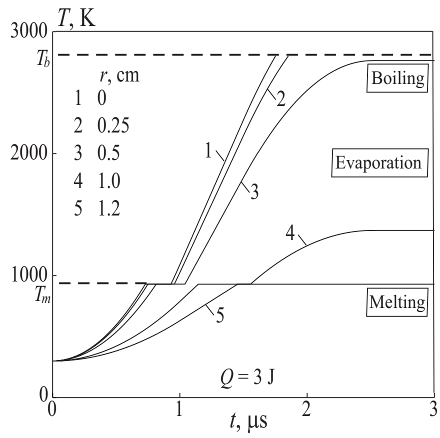

Figure 6. Temperature of metal particle.

Development of electron avalanche in the form of dependence of degree of ionization of vapour aureole on time is shown in the Figure 7. The particle is located on the centreline of laser beam. The electron avalanche is developed in 0.68 μs from the laser pulse started, and ionization takes place within a short time interval (it is about 0.04 μs).

The degree of ionisation as function of time and total energy of laser pulse is shown in the Figure 8. Microplasma spots around the particle are formed at energy of 1.03 J. Pre-breakdown conditions are sensitive to small change of energy of laser pulse. The threshold value of plasma formation is defined as a part of power passed up to the beginning of breakdown.

Interaction of laser pulse with individual metal particle is related to one of the following stages.

• Pre-threshold energy of laser pulse ($Q < 1$ J). Energy of laser pulse is not enough to ionize vapour aureole around particle. Evaporation of particle exists but degree of ionisation is small, and vapour aureole is transparent

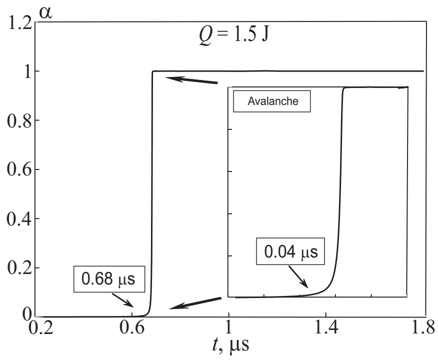

Figure 7. Development of electron avalanche.

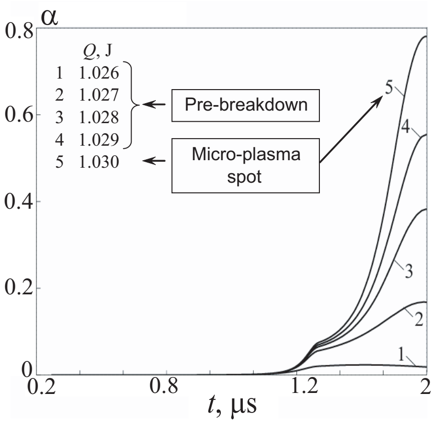

Figure 8. Degree of ionisation of vapour aureole.

for laser radiation.

• Near-threshold energy of laser pulse ($Q = 1$–2 J). Degree of ionisation changes from some percents to 100%.

• Post-threshold energy of laser pulse ($Q > 2$ J). The process proceeds at completely ionized vapour aureole around particle. Ionisation has an avalanche character within short time interval.

Liquid droplet. The temperature field in a water droplet and surrounding is shown in the Figure 9. The laser beam falls on the droplet from the right to the left. A local temperature rise is observed on the exposed surface of droplet. A thin thermal boundary layer is formed in the vicinity of the droplet. Increase in temperature inside droplet corresponds to the centre of internal vapour cavity which is located near shadow side of a droplet. The droplet is superheated and water is in the meta-stable state. Line 7 corresponds to the start of explosive process at temperature of 698 K. Time of explosive transformation of a droplet is 1.54 μs.

The plasma spot is non-transparent to radiation. Increase in pressure and temperature induces expansion of shock wave. Its intensity decreases with increase in distance from the centre of vapour cavity.

The Figure 10 shows the threshold value as a function of droplet radius. The time of optical breakdown is a result of the competition between 3 factors: (i) time of droplet heating to the temperature of explosive trans-

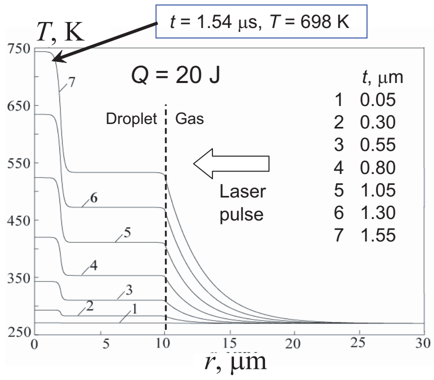

Figure 9. Temperature field inside and outside droplet.

formation (at low pulse energy, the large droplets do not have enough time for being heated, and the small droplets exchange heat intensively with the surrounding), (ii) intensity of the shock wave contributing to the thermal ionization of vapour (for massive droplets, the shock wave is weak), (iii) time of development of an electron avalanche.

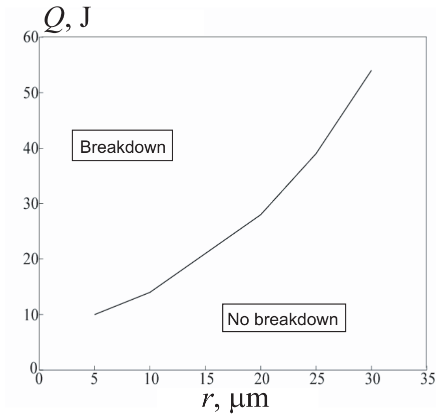

Figure 10. Threshold value on optical breakdown.

The size of the laser spot has a significant impact on the threshold value of optical breakdown. For droplets of 5 μm, a breakdown takes place at energy of 10 J. Increase in droplet radius leads to increase in time of droplet heating and decrease in degree of ionization. No electron avalanche develops at low intensity of laser pulse, and threshold value of optical breakdown increases.

Minimum pulse energy. The minimum pulse energy is a function of radius of laser spot, mass fraction of particulate component and volume fraction of oxidant.

The results obtained are presented in the Figure 11 for fish-plate aluminium particles in the acetylene–oxygen–nitrogen mixture. Volume fraction of acetylene is 15%. Volume fraction of oxygen changes from 15% to 35%. Mass fraction of particles is 1 g/m^3. Wave length of laser beam is 4.2 μm, radius of laser spot is 1.5 cm, and time of pulse is 2.6 μs [15, 16].

At $Q = 150$ J combustion of fuel takes place in small region adjacent to shock wave front. At $Q = 200$ J the temperature and pressure in shock wave front increase, and volume fraction of fuel decreases on 20–30% for time

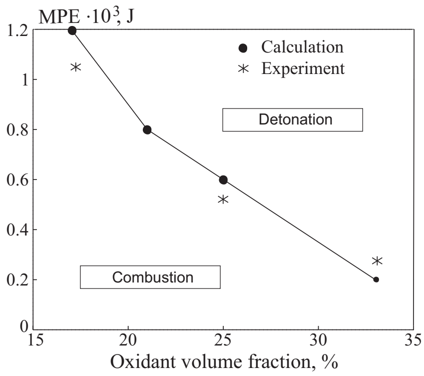

Figure 11. Minimum pulse energy of detonation.

of laser pulse. Further energy supply to mixture leads to considerable increase in temperature and pressure in the mixture, and development of unsteady gas dynamics processes in vapor aureole. At $Q = 300$ J about 60% of fuel is used, and at $Q = 300$ J about 95% of fuel burns beyond the shock wave front. The energy of laser pulse 350–400 J is the MPE of detonation.

Conclusions

The mathematical formulation of the problem was divided into low-level models and high-level models. The low-level models correspond to the processes in the volume occupied by an individual particle or droplet. The high-level models correspond to the processes in the volume occupied by the multi-phase mixture. The data obtained from solution of low-level problems are used to calculate source terms in the governing equations describing high-level model. The solution of high-level model provides volume fraction of particles and volume occupied by an individual particle or droplet.

The models of optical breakdown on the individual metal flake particle of non-spherical shape, and detonation of gas-particle mixture has been developed. The models takes into account heating and evaporation, formation of vapour aureole, generation of free electrons due to thermal ionization beyond the shock wave front, development of electron avalanche due to reverse drag effect and gas dynamics processes in the vapour aureole and the surrounding.

The threshold intensities of optical breakdown and minimum pulse energy of detonation in multi-phase mixture have been computed and contributing factors have been studied.

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