Laser-Induced Explosion and Detonation in Gas-Particle and Gas-Droplet Mixtures

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Outline

1. Introduction
2. Physical model
3. Mathematical model
4. Results
5. Conclusions

Introduction

Potential hazard — **Applications** — *Engineering solutions*

Equipment | Technology | Environment

Applied problems

Particulate reactive flows

Chemical reactions | Transport of particles | Heat and mass transfer

Combustion | Sub-models | Explosion/Detonation

Condensation, Evaporation, Complex morphology, Light absorption

Phase transitions | Thermal radiation

Fundamental problems

Computer simulation → Commercial/Open/In-house CFD codes

Theoretical analysis

Engineering analysis

Research methods

Experimental data

Optical Breakdown

Optical breakdown
When a laser radiation interacts with a gas, the gas breaks down and becomes highly ionized.

Pure gas or gas mixture → No free electrons → High intensity of laser pulse → $I_* = 10^{11}$ W/cm^2

Gas with particles or droplets → Vapor aureole → Free electrons → Low intensity of laser pulse → $I_* = 10^{9}$ W/cm^2

17% $CH_4 + O_2$, $t_p = 1$ μs, λ = 1 μm
Aluminium particles

Applied Problems

- Applications
  - Environmental monitoring of high-risk industrial objects and enclosed spaces
  - Measurements of flammability and explosibility limits in particulate reacting substances
  - Laser ignition of volumetric explosion for application to fire mitigation
  - Design of air-breathing pulse detonation engines
  - Technological processes

⇧

Minimum Pulse Energy
(MPE)

New Possibilities

- New possibilities
  - Lower intensity 10^9 W/cm^2 against 10^{11} W/cm^2
  - Distance ignition
  - No divergence of laser beam
  - Desired temporal and spatial distributions of ignition centres
  - Homogeneous ignition within sub-microsecond interval
  - Invariant gas-dynamical conditions over a large volume of mixture

Fundamental Problems

- Qualitative and quantitative description of the processes around individual particle/droplet
- Knowledge in particle microphysics and optical properties of particles
- Sub-models of heating and evaporation (particle type)
- Transport of aggregates of complex morphology
- Threshold values of optical breakdown
- Dependence of minimum pulse energy on the contributing factors (laser pulse, gas mixture, particles/droplets)
- Aero-optic effects

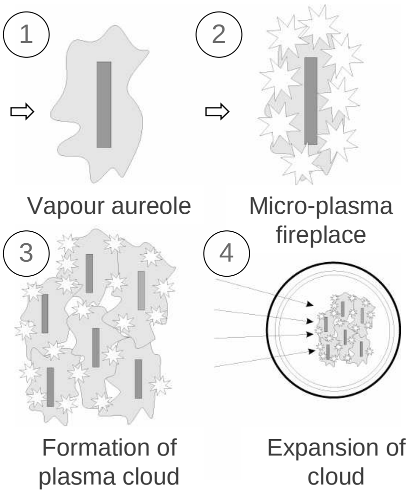
Objectives

- To develop physical and mathematical models and up-to-date numerical methodology for computer modeling
- To study laser-induced detonation in gas-dispersed mixtures and to demonstrate advantages of the new methodology
- To develop knowledge-based guidance in industry and to produce recommendations

Physical Model

- Qualitative description
- Sub-models
  - ❑ Individual particle/droplet } Micro-level
  - ❑ Multi-phase mixture } Macro-level

Metal Particle



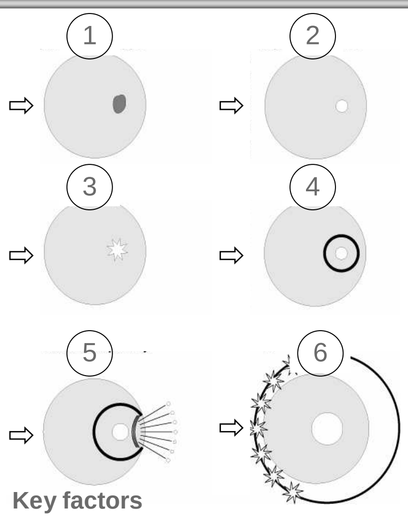
Physical model of development of optical breakdown in gas-particle mixture

Stages

1.
   - Heating, melting and evaporation
   - Formation of vapour aureole
2.
   - Ionisation of vapour aureole
   - Development of electron avalanche
   - Formation of micro-plasma fireplace
3.
   - Expansion of micro-plasma fireplaces
   - Formation of plasma cloud
4.
   - Development of shock wave
   - Initiation of detonation

Low evaporation temperature → Reverse drag effect → Breakdown **Key factors**

Liquid Droplet



Key factors

Internal vapour cavity ⟶ Breakdown

Physical model of development of optical breakdown in gas-droplet mixture

Stages

1 { • Focusing of radiation and rise of temperature

2 { • Overheating, formation of vapour cavity

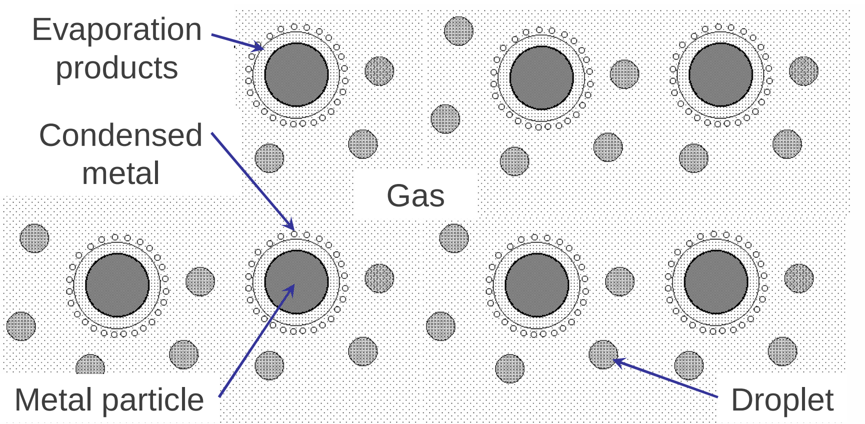
3 { • Internal micro-breakdown

4 { • Expansion of shock wave

5 { • Shock wave coming on shadow side
• Formation of micro-plasma fireplaces

6 { • Formation of micro-plasma aureole
• Expansion of shock wave
• Initiation of detonation

Multiphase Mixture



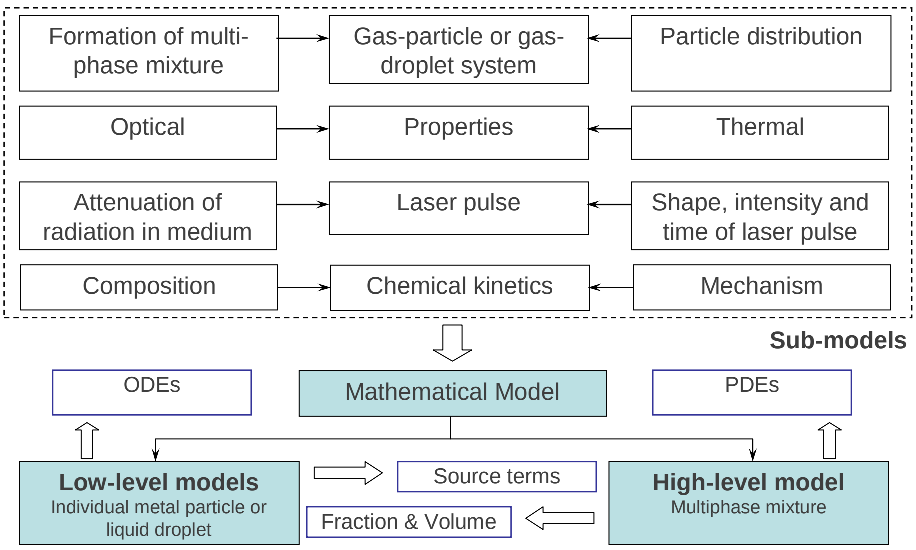
Gas	= Fuel + Oxidant + Combustion products + Neutral	Mixture Composition
Particulate	= Metal particles + Liquid droplets	
Vapor	= Neutral + Ions + Electrons	
Condensed	= Metal oxide	

Model Formulation

Features
- Multi-physical problem
- Wide range of temporal and spatial scales
- Correlation and interference of processes
- Non-spherical shape of metal particles

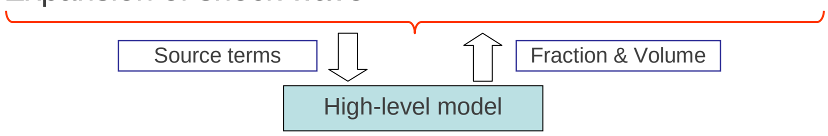
Requirements
- Co-ordination on accuracy
- Use of physical ideas
- Description of laser pulse (time, shape, energy)
- Model of real gas

Mathematical Model



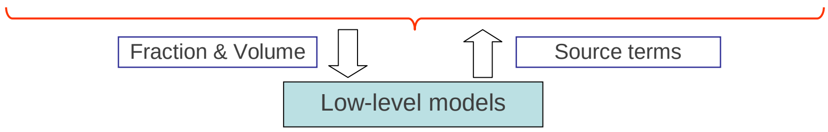
Low-Level Models

- Heating, evaporation, formation of vapour aureole
- Appearance of free electrons due to thermal ionisation on shock wave front
- Development of electron avalanche
  - Heating of vapour aureole due to electron and atom collisions
  - Heating of electron component
  - Ionisation of vapour aureole due to electron impact
  - Change of mass of particle
- Chemical reactions
- Expansion of shock wave



High-Level Model

- Eulerian approach
  (multi-velocity and multi-temperature continuum)
- Computational procedure
  - Finite volume method
    (model of real gas)
  - Splitting scheme on physical factors
    (Chakravarthy–Osher scheme)
  - Artificial pressure for particulate component
  - Monte Carlo method for thermal radiation transfer



Shape of Laser Pulse

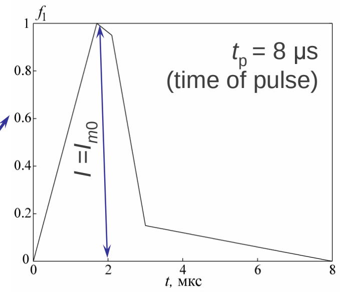
Intensity of laser pulse

$$I(t,x,y,z) = I_{m0} f_1(t) f_2(x,y) f_3(z)$$

Temporal distribution

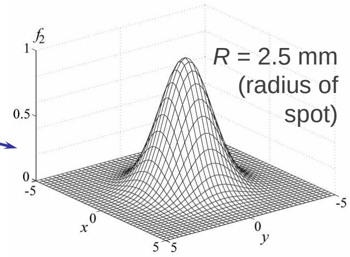
$$f_1(t) = \sum_{i=1}^{N-1} \left[F_i + (F_{i+1} - F_i) \frac{t - t_i}{t_{i+1} - t_i} \right] \phi(t_i, t_{i+1})$$

$$\phi(t_i, t_j) = \frac{t - t_i + |t - t_i|}{2|t - t_i| + \varepsilon} - \frac{t - t_j + |t - t_j|}{2|t - t_j| + \varepsilon}$$



Spatial distribution

$$f_2(x,y) = \exp\left[-\frac{2(x^2 + y^2)}{R^2} \right]$$



Absorption of radiation

$$f_3(z) = \exp(-\alpha z)$$

Energy of Laser Pulse

Total energy

$$Q_\Sigma = \int_0^\infty \int_0^\infty \int_0^\infty I(t,x,y)\, dx\, dy\, dt$$

$$Q_\Sigma = 2\pi I_{m0} S_\Sigma \frac{R^2}{4}$$

Integral time characteristic

$$S_\Sigma = \int_0^\infty f_1(t) dt = \frac{1}{2} \sum_{i=1}^{N-1} \frac{F_{i+1} + F_i}{t_{i+1} - t_i}$$

Laser pulse

t_p	= 2.6 μs	varies
λ	= 4.2 μm	chemical laser
R	= 5 mm	varies
S_Σ	= 1.5 μs	

Results

Processes

- Individual particle/droplet
- Dynamics of multi-phase mixture

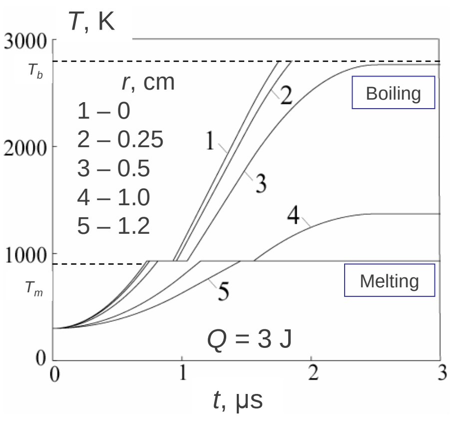
Factors

- Composition of mixture
- Particle orientation/location
- Total energy
- Time and shape of laser pulse

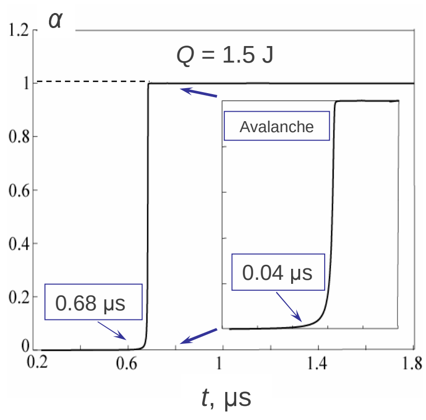
Quantities

- Threshold value of optical breakdown
- Minimum pulse energy

Metal Particle

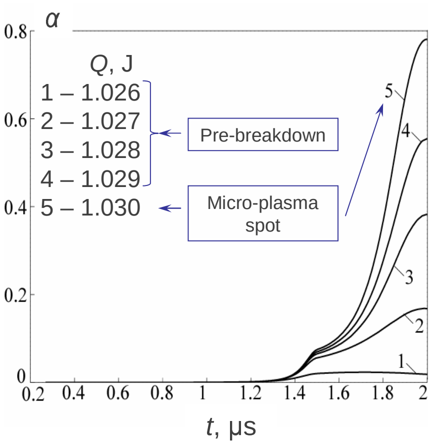


Time history of temperature of metal particle

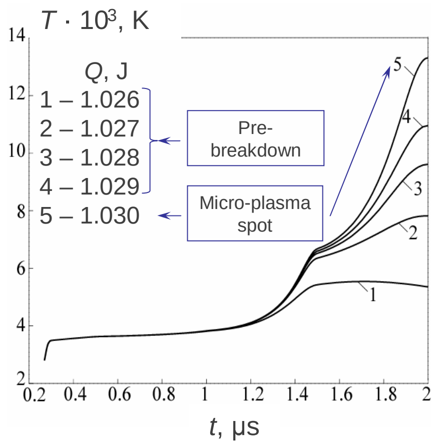


Time history of degree of ionisation of vapour aureole

Metal Particle



Time history of degree of ionisation of vapour aureole



Time history of temperature of electron component

Metal Particle

- Pre-threshold energy $Q < 1$ J

  α << 1

  - Energy is not enough to ionize vapour aureole
  - Evaporation exists, degree of ionisation is small
  - Vapour aureole is transparent for laser radiation

- Near-threshold energy $Q = 1–2$ J

  α ~ 1

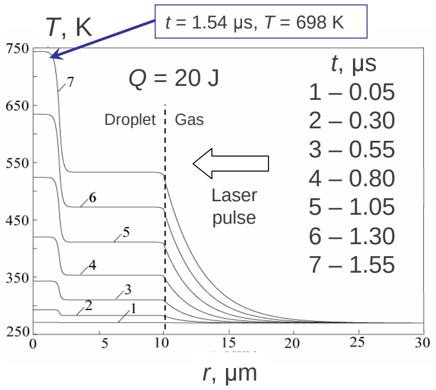
  - Degree of ionisation changes from some percents to 100%

- Post-threshold energy $Q > 2$ J

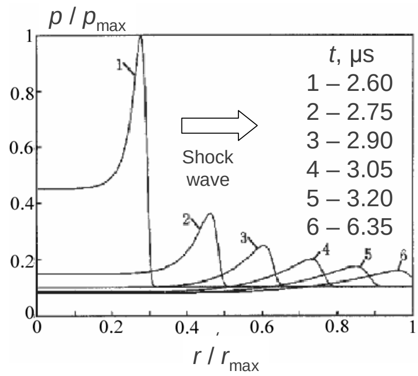
  α = 1

  - The process proceeds at completely ionized vapour aureole
  - Ionisation has an avalanche character within short time interval

Liquid Droplet

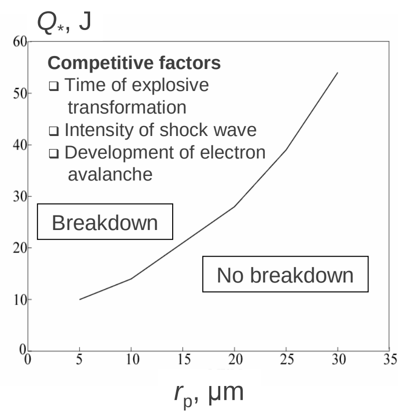


Temperature field inside and outside droplet



Pressure distribution in vapour aureole at the end of laser pulse

Liquid Droplet



Dependence of threshold value on size of droplet

t_e, T_e – time and temperature of explosive transformation

Breakdown conditions, $r_p = 5$ μm

Q, J	**t_e, μm**	**α**	**$T > T_e$**	**Yes/No**
5	–	–	–	–
10	1.83	10^{-2}	+	**+**
15	1.38	10^{-2}	+	+
20	1.13	10^{-2}	+	+
30	0.93	10^{-2}	+	+
50	0.72	10^{-2}	+	+

$r_p = 10$ μm

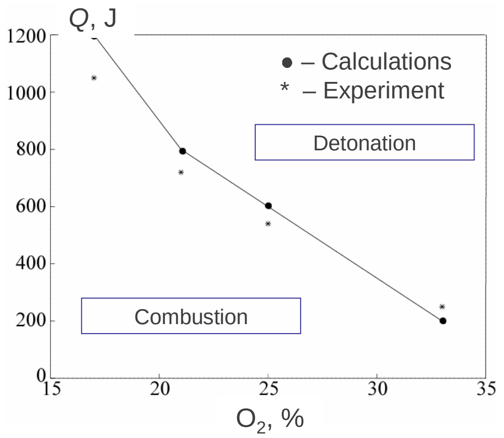
Q, J	**R, mm**
12	1.5
20	3
30	5

Laser spot

Breakdown conditions, $r_p = 20$ μm

Q, J	**t_e, μm**	**α**	**$T > T_e$**	**Yes/No**
5	–	–	–	–
10	–	–	–	–
15	1.48	10^{-11}	+	–
20	1.23	10^{-11}	+	–
30	1.04	10^{-11}	+	**+**
50	0.83	10^{-11}	+	+

Minimum Pulse Energy



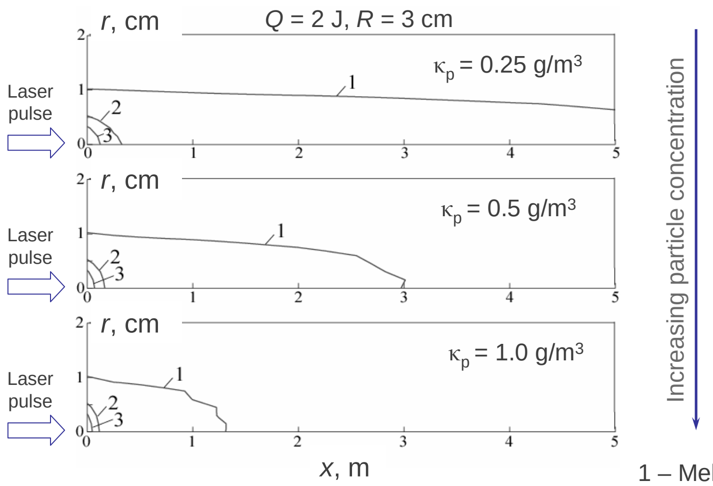
Dependence of minimum pulse energy on oxygen volume fraction

Mixture
C_2H_2 15%
O_2 (15–35)%
N_2

Particles
Aluminium
50 × 50 × 5 μm
κ_p = 1.0 g/cm³

Laser
λ = 4.2 μm
t = 2.6 μs
R = 1.5 cm

Specific Fronts



Location of specific fronts at the end of laser pulse

1 – Melting front
2 – Evaporation front
3 – Plasma formation front

Conclusions

- Contribution to theory
  - Multi-phase flows
  - Optical breakdown and detonation
- Tool of engineering analysis
  - Physical phenomena
  - Engineering solutions for industry
- Use in technology
  - Design and optimization of energy systems
  - Control of particle combustion
- Education
  - Course material
  - MSc/PhD programme

Future Work

- Nano-particles
- Molecular dynamics simulation

THANK YOU FOR YOUR ATTENTION!