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Numerical simulation of laser-induced detonation in mixture of hydrogen with suspended metal particles

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ABSTRACT

Simulation of interaction of laser pulse with gas–particle mixtures plays an important role in environmental and engineering applications. The injection of metal particles with low evaporation temperature and ionization potential causes optical breakdown on individual particle, and leads to drop of detonation minimum pulse energy in the mixture. The mathematical models and numerical methodology for computer modelling of optical breakdown and laser-induced detonation in gas–particle mixture are developed. Sub-models of optical breakdown on metal particle include heating of particle to boiling temperature, formation of vapour aureole around the particle, ionization of vapour aureole and development of electron avalanche, appearance of micro-plasma spots and their expansion, propagation of shock wave in the volume occupied by the particle. Laser-induced detonation in the mixture of hydrogen with flake aluminium particles is simulated based on Eulerian approach, and minimum pure energy of detonation is calculated for different parameters of laser pulse, mass fractions of particles and compositions of gas mixture.

1. Introduction

Hydrogen is increasingly used as an energy carrier in transport, stationary and other applications [1]. Detonation is a worst case scenario for accidents with unscheduled hydrogen release [2]. Risk assessment of hydrogen applications presents new challenges due to a large difference in properties of hydrogen and natural gas (reactivity, ignition energy, flammability and detonability limits, buoyancy, transport properties). Prediction of detonation parameters, as well as blast parameters beyond the detonation zone is important for hydrogen safety engineering, particularly for risk assessment through realistic safety distance assessment for hydrogen infrastructure and development of mitigation technologies.

Interaction of laser pulse with gas–particle mixtures plays an important role in different applications including environmental monitoring of high-risk industrial objects and enclosed spaces, measurements of flammability and explosibility limits in particulate reacting substances and propagation of laser radiation through explosive mixtures, laser-induced volumetric explosion for application to fire mitigation, design of air-breathing pulse detonation engines. Use of laser pulse allows to create desired temporal and spatial distributions of ignition centres and to perform a homogeneous

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Nomenclature

Latin symbols

a	pre-exponential factor
c	specific heat capacity, J/kg K
d	diameter, m
e	specific total energy, J/kg
f	function
k	Boltzmann constant, J/K
m	mass, kg
n	number density, $1/m^3$
p	pressure, Pa
q	heat release, J/kg
r	radius, m
t	time, s
u	velocity, m/s
$\mathbf{v}$	velocity, m/s
x,y,z	Cartesian coordinates, m
A	area, m^2
B	accumulative operating characteristics, J/m^2
C	constant, $m^6\ K^{9/2}/s$
C_D	drag coefficient
E	energy, J
F	flux
$\mathbf{F}$	source term in momentum equation
H	source term
I	intensity of laser pulse, W/m^2
J	source term in continuity equation, kg/m^3 s
K	absorption efficiency
N	number of ramp points
Nu	Nusselt number
Q	total energy of laser pulse, J
R	radius of laser spot, m
Re	Reynolds number
S	integral time parameter
T	temperature, K
U	conservative variables
V	volume, m^3
W	rate of chemical reaction, kg/m^3 s
Y	mass fraction, kg/m^3
Z	source term in energy equation

Greek symbols

α	degree of ionization
γ	ratio of specific heat capacities
β	equilibrium degree of ionization
ε	small parameter
ζ	absorption coefficient, 1/m
λ	thermal conductivity, W/m K
μ	absorption coefficient, 1/m
μ	dynamic viscosity, Pa s
ν	collision frequency, 1/s
ξ	progress variable
ρ	density, kg/m^3
ϕ	piecewise-linear function
φ	polar angle, rad
χ	volume fraction of particles
ω	reaction rate, kg/m^3 s

Subscripts

a	atom
b	boiling
e	electron
g	gas
k	ramp point
n	time layer
p	laser pulse
s	particle
v	vapour
0	initial
*	phase transition

Abbreviations

CFD	computational fluid dynamics
DDT	deflagration to detonation transition
CJ	Chapman–Jouguet
MPE	minimum pulse energy
ZND	Zeldovich–von Neumann–Doering

ignition within the sub-microsecond interval. Laser ignition has the potential to replace the conventional electric spark plugs in engines that are required to operate under much higher compression ratios, faster compression rates, and much leaner fuel-to-air ratios than engines today.

The role of particles in environmental and engineering applications is two-fold. On the one hand, particles may pose potential hazard for human activity (deposition of aerosols in human lungs). On the other hand, they can be successfully used in engineering solutions (to induce working processes in energy systems and to suppress detonation). Processes that control transport and combustion of particles remain unresolved, and introduce significant uncertainties into modelling and simulation. One of the most important parameters for engineering applications is the minimum pulse energy (MPE) required to induce detonation of the mixture.

The metal particles (typically aluminium) suspended in an oxidizing or combustible gas form a reactive gas–particle mixture. Reacting two-phase flows attract particular interest because of their applicability in various technological processes and energy conversion systems [3]. As a result, numerous investigations have been devoted to these flows.

Aluminized composite propellant contains a lot of aluminium particles because high combustion energy is generated and propulsion efficiency increases by burning aluminium particles. The high flame temperature of burning metal particles impacts large amounts of energy through the heat released during combustion. Many factors, such as the content and particle size of aluminium powders and its spatial localization, influence the combustion characteristics of these compositions.

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