Effects of particle diameter on the interactions between a circular particle cloud and hydrogen detonation wave

Yong Xu and Huangwei Zhang†

Department of Mechanical Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore, 117576, Republic of Singapore

1 Abstracts

Use of hydrogen (H_2) can reduce carbon emission, but H_2 leakage can induce hydrogen explosion and detonation. Chemically inert particle clouds can be used to mitigate hydrogen accidental explosions. This paper investigates a circular particle cloud interacting with a hydrogen detonation wave via the Eulerian—Lagrangian method with gas-particle two-way coupling. Different particle diameters are considered. Results show that particle size has a limited affecting on hydrogen detonation wave speed, but can significantly change the interphase transfer of energy and momentum, and particle cloud evolutions.

2 Introduction

Hydrogen is a decarbonized fuel that has lower ignition energy and wider flammability limit [1]. Therefore, leaked H_2 is prone to ignition and explosion. To inhibit accidental explosion of hydrogen, safety measures should be carefully implemented and evaluated. Chemically inert fine particles are one of the promising explosion inhibitors considering that they can be readily obtained and are also cheap and safe to be used without additional damage [2–4]. It has been shown that by implementing a particle curtain [2,3], the overpressure, propagation speed, and product gas temperature of detonation and/or blast waves can be effectively reduced, thereby minimizing the damage to surrounding infrastructure and personnel.

The influence of inert particle curtains on the detonation wave (DW) has been extensively studied [5–8]: composition and distribution of the particles [9,10] and particle size and concentration [2,11–17]. Existence of a particle curtain may induce unsteadiness in detonation propagation. Different DW propagation modes include detonation extinction and transmission [5,12,13,18–20], and instantaneous extinction followed by detonation re-initiation [14,16–19] and a galloping detonation near the flammability limit [12,13,20], are also explored. However, the underlying mechanisms behind these transient detonation dynamics have not been clarified, particularly in terms of the interactions between the detonation wave and solid particles and evolutions of particle cloud morphology.

In this work, detailed simulations with the Eulerian—Lagrangian approach and two-way gas-particle coupling are conducted to simulate the interactions of hydrogen detonation with circular cloud of dilute inert particles. The objectives of this paper include: (1) interactions between gas and particles; and (2) evolution of curtain morphology in detonated flows.

Correspondence to: huangwei.zhang@nus.edu.sg

3 Physical problem

A circular particle cloud interacting with a detonation wave is simulated in a two-dimensional configuration, as shown in Fig. 1. The computational domain is 0.3 m × 0.025 m, which includes a detonation development section ($0 \leq x < 0.2$ m) and a two-phase section ($0.2 \leq x \leq 0.3$ m). The domain is initially filled with stoichiometric H_2/air mixture. The initial temperature and pressure are $T_0 = 300$ K and $p_0 = 0.05$ MPa, respectively. The domain sections 0—0.1m and 0.1—0.3 m are respectively discretized by uniform Cartesian cells of 0.16×0.16 and 0.08×0.08 mm^2. The detonation is initiated by three vertically placed hot spots (2,000 K and 5 MPa) near the left end ($x = 0$ m), as plotted in Fig. 1. For the left boundary ($x = 0$), a non-reflective condition is enforced for the pressure, while a zero-gradient condition for other quantities. Zero-gradient condition is applied at $x = 0.3$ m and the upper and lower boundaries are set to be periodic. The radius of the particle cloud R is 0.0125 m, corresponding to 50% of the domain width W. Inside the cloud, mono-sized inert solid particle (diameter d_p = 5, 20, 50 µm, and concentration $c = 1$ kg/m^3) are uniformly distributed. They are static ($u_p = 0$) before the detonation wave arrives. Their initial temperature, material density and heat capacity are 300 K, 2,500 kg/m^3 and 900 J/kg·K, respectively.

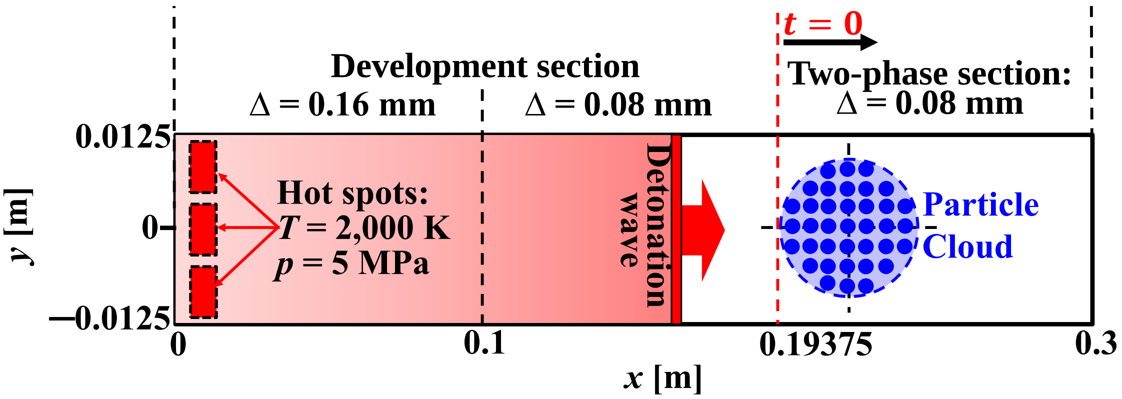

Figure 1: Schematic of the computational domain. The blue dots represent particles. Domain and particle sizes not to scale.

4 Mathematical model

The governing equations of mass, momentum, energy, and species mass fraction are solved with the ideal gas equation of state. The Lagrangian method is used to track a number of spherical solid particles in the dispersed phase. The interactions between the particles are neglected because we only study the dilute particle cloud with the initial particle volume fraction being generally less than 0.1% [21]. Only the Stokes drag is considered [22], and the convective heat transfer is modelled using the Ranz-Marshall correlation [23]. Computational parcel is used in our simulations to represent a series of solid particles with similar properties (e.g., temperature, diameter, and movement). The gas and liquid phase governing equations are solved by a compressible two-phase reacting flow solver, *RYrhoCentralFoam* [24–26]. The hydrogen mechanism with 13 species and 27 reactions [27] is used. For the particle phase, the particles are tracked based on their barycentric coordinates. The simulations run with 3,840 processors of the Fugaku Cluster from the RIKEN Center for Computational Science in Japan. The physical time of 100 microsecond can be achieved with wall clock time of approximately 22 hours.

5 Results and discussions

5.1 Gas phase

Figure 2 quantifies the evolutions of the lead shock speed D_{SF}, which are scaled by the C—J velocity D_{CJ} (1,961 m/s) of particle-free hydrogen/air mixture. A slightly reduced shock speed is observed with the 20 and 50 μm, and after the shock leaves the cloud, it is gradually restored to approximately the initial value. When the DW crosses the smaller particle cloud (5 μm), the velocity drops to below 95% D_{CJ} around x = 0.22-0.23 m. Thereafter, D_{SF} rises to about the 0.98 C—J speed at around x = 0.24 m. Nonetheless, when c = 1 kg/m^{3}and R = 0.25 W, all the shock speeds are insignificantly influenced by the particle diameter. This may be due to the lower particle concentration. In the future, we will conduct a series of parametric studies, such as higher concentration and/or larger cloud diameter.

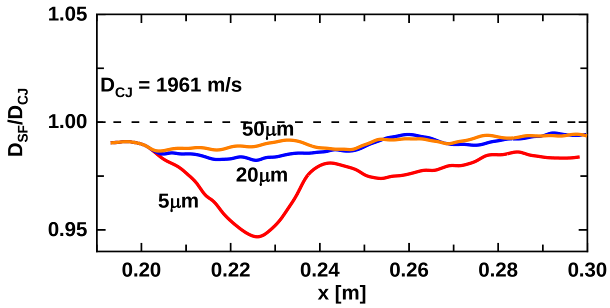

Figure 2: Influence of the particle diameter on the shock speeds of hydrogen detonation wave, scaled by the C—J value of pure gas mixture. c = 1 kg/m^3.

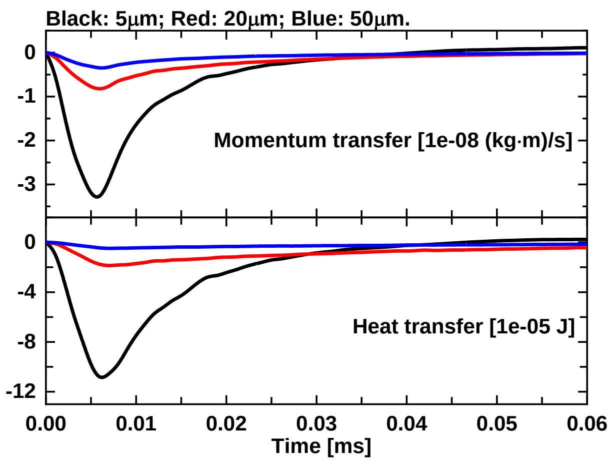

Figure 3: Influence of the particle diameter on the interphase transfer of momentum and heat. c = 1 kg/m^3.

5.2 Two-phase interaction

The interphase transfer of energy and momentum from Fig. 2 are plotted in Fig. 3. Both transfer are calculated based on the domain (x = 0 – 0.3 m). A negative value indicates that the energy or momentum is transferred from the gas to particles. One can see from Fig. 3 that the magnitudes of both energy and momentum transfer rates first increase and subsequent decrease. The increase is induced by more particles in the post-detonation area as the DW travels in the cloud. Subsequently, the thermal and velocity equilibria between the gas and particles are achieved, and interphase exchanges gradually decrease. Beyond a critical time, for instance, 0.03 ms, both transfer approach zero. It is observed that

5 μm has the highest peak values of energy/momentum transfer due to its larger specific surface area and smaller particle momentum and thermal relaxation time.

5.3 Particle phase

Here we discuss the effects of the particle diameter on the evolutions of cloud morphology colored with particle *x*-direction velocity $u_{p,x}$, plotted in Figs. 4—5. Their particle conditions are c = 1 kg/m^3, d_p = 5 and 50 μm, respectively. At 0 ms, the particle cloud is intact and stationary before the DW arrives. At 0.05 ms, the DW has passed through the cloud. Due to the detonation impacting, cloud particles are shocked and accelerated, and gradually move with the shock, which leads to a shrinking cloud. Closer inspection of 0.05 ms shows that some jets of shocked particles appear near the southern/northern poles of the cloud. This phenomenon is caused by the fast response of the fine particles to the local aerodynamics, i.e., vortex shedding due to the impulsive shock acceleration of a perturbed interface between multiphase fluids [28,29]. Meanwhile, at 0.05 ms, the evolutions of vortices further lead to two tails of particles extending from the cloud. At the subsequent instants, e.g., 0.09-0.31 ms, these tails are continuously stretched relative to the cloud. However, different form the results of Fig. 4, no tails of particles growing from the cloud are observed from Fig. 5. Meantime, the particle distribution range is much smaller than that of the 5 μm case. This is because larger particles result in longer momentum transfer timescale, leading to lower velocity difference between the gas phase and particle cloud.

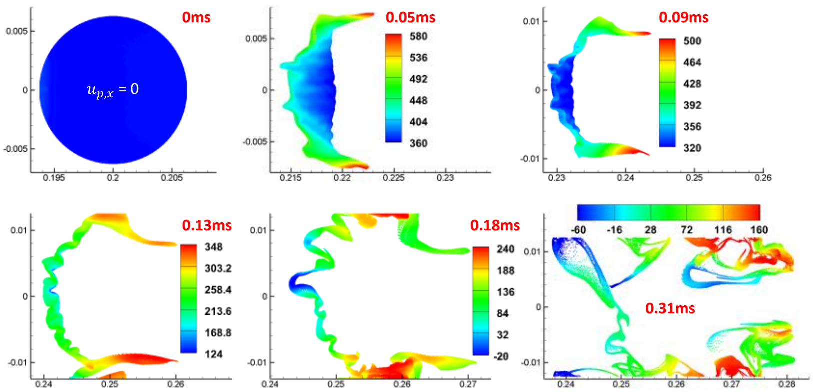

Figure 4: Time history of particle cloud morphology. c = 1 kg/m^3 and d_p = 5 μm. Axis label unit: m.

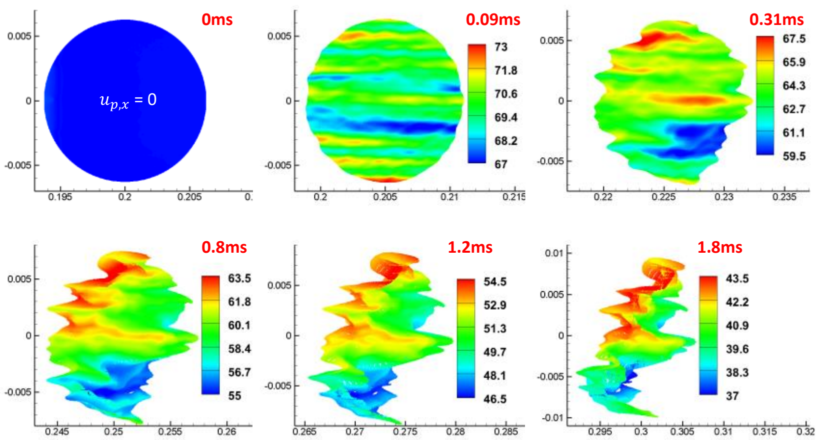

Figure 5: Time history of particle cloud morphology. c = 1 kg/m^3 and d_p = 50 μm. Axis label unit: m.

6 Conclusion

Interactions between a propagating hydrogen detonation wave and circular particle cloud are simulated by Eulerian-Lagrangian method and detailed chemical mechanism. The results show that particle size have limited effects on the shock speed when the concentration is fixed to be 1 kg/m^3. However, the diameter effects on the interphase exchange can be clearly observed. In addition, mechanism of particle cloud evolution is demonstrated with the time history of Lagrangian particle distributions. It is confirmed that particle size (5 μm and 50 μm) have significant influence on the cloud morphology. Analysis shows that smaller diameter would lead to wider particle dispersion range due to formation of vortices.

Acknowledgement

Here we use the Fugaku computing resource (Project hp210325). This work is supported by Singapore Ministry of Education Research Grant (A-8000199-01-00).

References

[1] Olmos F, Manousiouthakis VI. (2013). Hydrogen car fill-up process modeling and simulation. Int. J. Hydrogen Energy. 38:3401.

[2] Fomin PA, Chen JR. (2009). Effect of chemically inert particles on thermodynamic characteristics and detonation of a combustible gas. Combust. Sci. Technol. 181:1038.

[3] Liu Q, Hu Y, Bai C, Chen M. (2013). Methane/coal dust/air explosions and their suppression by solid particle suppressing agents in a large-scale experimental tube. J. Loss Prev. Process Ind. 26:310.

[4] Song Y, Nassim B, Zhang Q. (2018). Explosion energy of methane/deposited coal dust and inert effects of rock dust. Fuel. 228:112.

[5] Kratovaa YV, Fedorova AV. (2014). Interaction of a heterogeneous detonation wave propagating in a cellular regime with a cloud of inert particles. Combust. Explos. Shock Waves. 50:183.

[6] Khmel' TA, Fedorov AV. (2014). Modeling of propagation of shock and detonation waves in dusty media with allowance for particle collisions. Combust. Explos. Shock Waves. 50:547.

[7] Liu Y, Liu X, Li X. (2016). Numerical investigation of hydrogen detonation suppression with inert particle in pipelines. Int. J. Hydrogen Energy. 41:21548.

[8] Tahsini, AM. (2016). Detonation wave attenuation in dust-free and dusty air. J. Loss Prev. Process Ind. 39:24.

[9] Fedorov AV, Kratova YV. (2015). Influence of non-reactive particle cloud on heterogeneous detonation propagation. J. Loss Prev. Process Ind. 36:404.

[10] Fedorov AV, Kratova YV. (2015). Analysis of the influence of inert particles on the propagation of a cellular heterogeneous detonation. Shock Waves. 25:255.

[11] Fedorov AV, Tropin DA, Bedarev IA. (2010). Mathematical modeling of detonation suppression in a hydrogen-oxygen mixture by inert particles. Combust. Explos. Shock Waves. 46:332.

[12] Tropin DA, Fedorov AV. (2018). Attenuation and Suppression of Detonation Waves in Reacting Gas Mixtures by Clouds of Inert Micro- and Nanoparticles. Combust. Explos. Shock Waves. 54:200.

[13] Tropin D, Fedorov A. (2019). Physical and mathematical modeling of interaction of detonation

waves in mixtures of hydrogen, methane, silane, and oxidizer with clouds of inert micro-and nanoparticles. Combust. Sci. Technol. 191:275.

[14] Fedorov AV, Tropin DA. (2013). Modeling of detonation wave propagation through a cloud of particles in a two-velocity two-temperature formulation, Combust. Explos. Shock Waves. 49:178.

[15] Tropin DA, Fedorov AV. (2014). Physicomathematical modeling of detonation suppression by inert particles in methane-oxygen and methane-hydrogen-oxygen mixtures. Combust. Explos. Shock Waves. 50:542.

[16] Tropin DA, Fedorov AV. (2014). Mathematical modeling of detonation wave suppression by cloud of chemically inert solid particles. Combust. Sci. Technol. 186:1690.

[17] Pinaev AV, Vasil'ev AA, Pinaev PA. (2015). Suppression of gas detonation by a dust cloud at reduced mixture pressures. Shock Waves. 25:267.

[18] Gottiparthi KC, Menon S. (2012). A study of interaction of clouds of inert particles with detonation in gases. Combust. Sci. Technol. 184:406.

[19] Fedorov AV, Kratov YV. (2013). Calculation of detonation wave propagation in a gas suspension of aluminum and inert particles. Combust. Explos. Shock Waves. 49:335.

[20] Tropin DA, Bedarev IA. (2021). Problems of detonation wave suppression in hydrogen-air mixtures by clouds of inert particles in One- and Two-dimensional formulation. Combust. Sci. Technol. 193:197.

[21] Crowe C, Schwarzkopf J, Sommerfeld M, Tsuji Y. 2011. Multiphase Flows with Droplets and Particles, 2nd ed., CRC Press.

[22] Liu AB, Mather D, Reitz RD. (1993). Modeling the effects of drop drag and breakup on fuel sprays. SAE Tech. Pap. 83.

[23] Ranz WE, Marshall WR. (1952). Evaporation from Drops, Part I. Chem. Eng. Prog. 48:141.

[24] Huang Z, Zhao M, Xu Y, Li G, Zhang H. (2021). Eulerian-Lagrangian modelling of detonative combustion in two-phase gas-droplet mixtures with OpenFOAM: Validations and verifications. Fuel. 286:119402.

[25] Xu Y, Zhao M, Zhang H. (2021). Extinction of incident hydrogen/air detonation in fine water sprays. Physics of Fluids. 33:116109.

[26] Xu Y, Zhang H. (2022). Pulsating propagation and extinction of hydrogen detonations in ultrafine water sprays. Combust. and Flame. 241:112086.

[27] Burke MP, Chaos M, Ju Y, Dryer FL, Klippenstein SJ. (2012). Comprehensive H_2/O_2 kinetic model for high-pressure combustion. Int. J. Chem. Kinet. 44:444.

[28] Vorobieff P, Anderson M, Conroy J, White R, Truman CR, Kumar S. (2011). Vortex formation in a shock-accelerated gas induced by particle seeding. Phys. Rev. Lett. 106:184503.

[29] Duke-Walker V, Maxon WC, Almuhna SR, McFarland JA. (2021). Evaporation and breakup effects in the shock-driven multiphase instability. J. Fluid Mech. 908:A13.