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# Numerical Analysis of the Mean Structure of Gaseous Detonation with Dilute Water Spray

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Two-dimensional (2D) numerical simulations based on Eulerian-Lagrangian method that take droplet breakup into account are conducted to clarify the mean structure of gaseous detonation laden with a dilute water spray. The premixed mixture is a slightly diluted stoichiometric hydrogen oxygen mixture at low pressure. The simulated results are analyzed via 2D flow fields and statistical Favre spatiotemporal average technique. Gaseous detonation with water droplets (WDs) propagates stably with a velocity decrease compared with the dry Chapman-Jouguet speed. The mean structure of gaseous detonation with dilute water spray shares similar structure as the one without water spray. However, the hydrodynamic thickness is changed due to the interaction with water spray. Overall interphase exchanges (mass, momentum and energy) that take place within the hydrodynamic thickness induce a decrease of the detonation velocity and lower the level of fluctuations downstream of the mean leading shock wave. Droplet breakup occurs downstream of the induction zone and in our case, the water vapor from the evaporation of water spray does not affect the reactivity of gaseous detonation. The laminar Master Equation for gaseous detonation laden with inert WDs shows that the hydrodynamic thickness should rely on the gaseous sound speed, and works well as the working mixture is weakly unstable and its cellular structure is regular. The droplet flow regimes and breakup modes have also been determined. The characteristic lengths of detonation and interphase exchanges have been ordered under the present simulation conditions and have been shown to be intimately intertwined.

**Key words:**

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## 1. Introduction

Since its discovery, detonation phenomena have attracted a lot of attention regarding safety hazards and propulsion applications. Detonation is a self-sustaining supersonic premixed combustion wave, which consists of a leading shock wave coupled with a reaction zone.

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Many advantages could be achieved from its use in a combustor. Indeed, according to the Fickett-Jacob cycle, higher total temperature and pressure than in conventional engines can be reached, resulting in a higher thermal efficiency and increased thrust. Moreover, the use of smaller compressors renders the engine more compact. These reasons have motivated many studies all over the world (Kailasanath 2000; Roy *et al.* 2004; Wolanski 2013). As the full-scale propulsion system is limited in space, using fuel as a liquid is very attractive because of its high energy density content (see Li *et al.* 2011; Lu *et al.* 2017 on liquid fuel based pulsed detonation engines and Kindracki 2015; Frolov *et al.* 2017 for rotating detonation engines). For instance, Kindracki (2015) designed the geometry of a rotating detonation chamber that uses liquid kerosene and gaseous air and investigated the initiation and propagation of rotating detonation. No stable rotating detonation could be obtained at room temperature. Stable operation were then obtained with lean and rich mixtures, with a small addition of gaseous hydrogen (below the lean limit) and 20% liquid isopropyl nitrate. A velocity deficit of 20-25% as compared to the Chapman-Jouguet (CJ) velocity was furthermore observed. Moreover, the instability of the detonation wave with liquid fuel may affect the performance and reliability of detonation engine and therefore must be controlled.

On the other hand, a severe damage to people and goods may occur if the detonation happens unintentionally, such as in coalmines or nuclear power plants. Therefore, the knowledge on initiation and mitigation of detonations are essential for safety applications. One of the potential solutions to mitigate the damages is the use of water sprays (Thomas 2000). Boeck *et al.* (2015) showed that water droplets whose Sauter mean diameter (SMD) is 13  $\mu\text{m}$  delays the deflagration-to-detonation transition for atmospheric stoichiometric hydrogen air mixture and that the detonation propagation speed decreases by 3% as compared to the CJ speed. Another experimental study by Niedzielska *et al.* (2017) indicated the possibility of water spray with SMD of 500  $\mu\text{m}$  for detonation quenching.

Therefore, knowledge on detonation in liquid heterogeneous mixture is of primary importance (Murray & Thibault 2009; Higgins 2012) not only for the development of the detonation combustor using liquid fuel but also for the mitigation of detonation by water spray. Many fundamental researches (Ragland, Dabora & Nicholls 1968; Dabora, Ragland & Nicholls 1969; Thomas, Edwards & Edwards 1990; Ju & Law 2002; Chang & Kailasanath 2003; Lu & Law 2004; Papalexandris 2004; Papalexandris 2005; Kailasanath 2006; Smirnov *et al.* 2007; Fedorov & Kratova 2015a; Fedorov & Kratova 2015b; Jarsalé, Virot & Chinnayya 2016; Benmahammed *et al.* 2016; Liu, Liu & Li 2016) have been conducted to obtain some physical insight into these combined phenomena. Their aim is to clarify their characteristics such as lower propagation velocity compared with the CJ velocity, modification of the cellular structures, and delayed (or enhanced) deflagration-to-detonation transitions. In addition, these aforementioned characteristics are known to be affected by the droplet diameter, liquid volume fraction, polydisperse droplet diameter distribution and mixture reactivity. Nevertheless, the detailed propagation mechanism and the structure of gaseous detonation in heterogeneous mixtures remain partially understood as compared to homogeneous gaseous detonation.

One of the studies to clarify the structure for gaseous detonation with water droplets (WDs) in term of the hydrodynamic thickness has been conducted by Jarsalé, Virot & Chinnayya (2016). They performed an experiment to generate new data on gaseous detonation propagating through a  $\text{C}_2\text{H}_4$ -air mixture laden with WDs. The cell size was drastically altered and the velocity decreased compared with the dry CJ velocity. Also, they measured the hydrodynamic thickness by the analysis of the post-shock pressure fluctuations and revealed that the ratio of hydrodynamic thickness over the cell size remains quite constant regardless of the presence of WDs. However, they were not able

to get access to the behavior of WDs such as for instance their motion and the location of evaporation. Therefore, both numerical and experimental approaches are required to understand the structure of detonation in heterogeneous mixtures and the interplay between phases. Watanabe *et al.* (2019) performed two-dimensional (2D) numerical simulations based on previous experiments by Jarsalé, Virost & Chinnayya (2016) and analyzed the structure of two-phase detonation via Favre averaged one-dimensional profiles. Favre averaging of gaseous detonations has been previously performed to gain more insight into the chaotic and turbulent cellular gaseous detonations (Radulescu *et al.* 2007; Lee & Radulescu 2005; Maxwell *et al.* 2017), when losses are present (Reynaud, Virost & Chinnayya 2017; Sow, Chinnayya & Hadjadj 2014; Sow, Chinnayya & Hadjadj 2015; Sow, Chinnayya & Hadjadj 2019) and with spatially inhomogeneous initial conditions (Mi, Timofeev & Higgins 2017; Mi *et al.* 2017). Watanabe *et al.* (2019) confirmed stable propagation of gaseous detonation in fresh gas mixture with WDs with a small velocity decrease (maximum 3.2%) as compared to the dry CJ speed and also the change of the cellular structure by addition of WDs in the leaner mixture case as in the experiments. The structure of detonation can be seen to be significantly modified by WDs evaporation. This endothermic process is coupled with the detonation wave and the levels of velocity, vorticity and temperature fluctuations downstream of the mean leading shock are lowered. Additionally, they reported that the hydrodynamic thickness decreased with WDs when the sound speed for two-phase mixture of which one of the assumptions is velocity equilibrium, is used. Nevertheless, the computational domain was quite short from the interaction with water droplet domain (i.e., 100 mm). Moreover, their Favre average analysis was based only on one last instantaneous flow field of the gaseous phase and they did not obtain the dispersed phase counterpart. In addition, they did not take into account droplet breakup. Indeed, the impingement of high amplitude shock wave on the liquid dispersed phase will shatter the droplets. The exchange surface will be increased and will enhance the energy transfer between phases.

Steady laminar detonation is composed of a shock wave, followed by an induction zone where a pool of intermediate species proliferate before the exothermic reactions proceed to raise the temperature. However, detonations are intrinsically unstable and are prone to develop multidimensional cellular structures, of which regularity depends on the reactivity of the mixture. These instabilities delay the mean sonic line, propagating at the same speed as the shock and which isolates the detonation front from the rear. Thus, four characteristic lengths of detonation can be defined at least (Lee 2008): induction and reaction lengths, the cell size and the hydrodynamic thickness, which is the distance from the mean shock to the mean sonic plane.

After the passage of the shock that is driven by the gas phase in the dilute regime, the mixture is out of equilibrium. At least, three relaxation zones (in contrast to two with solid particles) can be identified to recover this equilibrium: droplet equilibration to the saturation temperature, velocity and temperature equilibration (Guha 1992). As the shock is of high amplitude in detonation conditions, breakup is likely to occur, which will enhance the relaxation processes and its characteristic time has to be taken into account (Kolev 2007; Saurel & Lemetayer 2001). Secondary atomization is a very active field of research (Guildenbecher, Lopez-Rivera & Sojka 2009). More recently, Theofanous (2011) has discussed the different physical mechanisms that could explain the loss of the integrity of the droplet. The present study is also motivated by Jarsalé's experiments (Jarsalé 2017), driven by the ratio of the induction length to the secondary breakup length of the spray of droplets.

Therefore, this study aims to understand to which extent the four detonation characteristic lengths and the four droplet characteristic times can be intertwined, and how these

processes interact with each other. To that end, a weakly unstable gaseous mixture with an initial regular cellular structure is chosen, for which the third dimension should not bring any quantitative difference on the mean quantities (Taileb *et al.* 2018). The mixture is  $2\text{H}_2 + \text{O}_2 + 2\text{N}_2$  at the initial low pressure of 10 kPa and at an initial temperature of 300 K. The mass loading of the water droplets is 0.07, with a uniform diameter of 15.9  $\mu\text{m}$ . This initial distribution is expected to evolve as the droplet undergoes continuous acceleration as well as transverse shock wave impingement during its course within the cell. In addition, the different flow and breakup regimes that the droplet undergoes from the shock to the mean sonic plane can also be inferred from the computations.

In order to capture the motion and behavior of WDs, an Eulerian-Lagrangian method is desirable to model the two-phase mixture. In addition, the evaporation of WDs generates additional water vapor in the gaseous phase and the reactivity of the mixture may thus be affected. Therefore, in this study, two-dimensional numerical simulations based on Eulerian-Lagrangian method that takes droplet breakup into account and reactive Navier-Stokes equations, with source terms accounting for the detailed chemistry and the interactions with the liquid phase are performed to clarify quantitatively the influence of the dilute water spray on the characteristics of the gaseous detonation. Detailed discussion is carried out to analyze the detonation structure and the interactions between gas phase and water spray via statistical Favre averaged one-dimensional profiles for both gaseous phase and dispersed phase from the simulation results. The recycling block method (Sow, Chinnayya & Hadjadj 2019) is used to enable longer length of the detonation propagation.

The plan of this paper is organized as follows. Section 2 describes the mathematical modeling and numerical method for gaseous detonation with dilute water spray. Then, the problem statement is presented in Section 3. Section 4 presents the results obtained in the simulation and discusses the mean structure of gaseous detonation with dilute WDs. The different flow regimes of the droplet will be highlighted. A Master Equation will be derived, that helps to classify the relative importance of the different interphase exchanges to the thermicity. The effect of the evaporated water on the reactivity of the mixture will also be evaluated. Finally, the main conclusions are drawn in Section 5.

## 2. Mathematical modeling and numerical method

### 2.1. Governing equations

The detonation propagation in a water spray is related to two-phase flow of gas and liquid droplets. The Eulerian-Lagrangian method is used to model the gaseous detonation laden with dilute water spray. The gaseous phase is assumed to be a viscous, reactive, compressible, and ideal gas. Nine chemical species are considered, namely  $\text{H}_2$ ,  $\text{O}_2$ ,  $\text{H}$ ,  $\text{O}$ ,  $\text{OH}$ ,  $\text{H}_2\text{O}$ ,  $\text{HO}_2$ ,  $\text{H}_2\text{O}_2$  and  $\text{N}_2$ . The governing equations combined with gas porosity are the 2D reactive compressible Navier-Stokes equations with source terms accounting for the chemical reactions and the interactions with the droplets. The equation of state for

an ideal gas is used to close the system.

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g) = \frac{1}{V_{\text{cell}}} \sum_{i=i_1}^{i_2} n_i \dot{m}_i \quad (2.1)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g \mathbf{u}_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g \mathbf{u}_g) - \nabla \cdot (\alpha_g \boldsymbol{\tau}_g) + \alpha_g \nabla p_g = \frac{1}{V_{\text{cell}}} \sum_{i=i_1}^{i_2} n_i [\dot{m}_i \mathbf{u}_i - \mathbf{f}_{\text{drag},i}] \quad (2.2)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_g e_g) + \nabla \cdot [\alpha_g (e_g + p_g) \mathbf{u}_g] - \nabla \cdot (\alpha_g \boldsymbol{\tau}_g \mathbf{u}_g) - \nabla \cdot (\alpha_g q_g) + p_g \frac{\partial \alpha_g}{\partial t} \\ = \frac{1}{V_{\text{cell}}} \sum_{i=i_1}^{i_2} n_i \left[ \frac{1}{2} \dot{m}_i \mathbf{u}_i \cdot \mathbf{u}_i - \mathbf{f}_{\text{drag},i} \cdot \mathbf{u}_i - (q_{\text{conv},i} + q_{\text{evap},i}) \right] \end{aligned} \quad (2.3)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g Y_{g,k}) + \nabla \cdot [\alpha_g \rho_g Y_{g,k} \mathbf{u}_g] - \nabla \cdot (\alpha_g \mathbf{j}_{g,k}) = \alpha_g \dot{\omega}_{g,k} + \frac{1}{V_{\text{cell}}} \sum_{i=i_1}^{i_2} n_i \dot{m}_{i,k} \quad (2.4)$$

$$p_g = \rho_g R_g T_g \quad (2.5)$$

Here,  $\alpha_g$ ,  $\rho_g$ ,  $\mathbf{u}_g$ ,  $p_g$ ,  $T_g$ ,  $e_g$ ,  $Y_{g,k}$  and  $R_g = R_u (\sum_{k=1}^{N_s} Y_{g,k}/W_g)$  represent porosity, gas density, velocity vector, pressure, temperature, total energy, mass fraction of species  $k$  and gas constant, respectively.  $N_s$  is the total number chemical species.  $\boldsymbol{\tau}_g$ ,  $q_g$ ,  $\mathbf{j}_{g,k}$  and  $\dot{\omega}_{g,k}$  denote the shear stress, heat flux, diffusion flux, and reaction rate, respectively.  $V_{\text{cell}}$ ,  $n_i$ ,  $\mathbf{f}_{\text{drag},i}$ ,  $q_{\text{conv},i}$ ,  $q_{\text{evap},i}$  and  $\dot{m}_i$  are cell volume, number density, drag force, heat flux by convection, heat flux by evaporation, and mass flux by evaporation, respectively for each droplet  $i \in (i_1, i_2)$  belonging to the cell volume.

The hydrogen-oxygen combustion mechanism used is the detailed model proposed by Hong, Davidson & Hanson (2011), which considers 9 species and 20 elementary reactions. The detailed chemical mechanism is given in Appendix A. The thermochemical species properties are calculated using the JANAF thermochemical polynomials (McBride, Gordon & Reno 1993). As for the transport properties of viscosity and thermal conductivity but for  $\text{HO}_2$ , a method proposed by Gordon, McBride & Zeleznik (1984) is used to estimate the gas viscosity and thermal conductivity. The reason why the transport coefficients of viscosity and thermal conductivity are evaluated using the different methods is that the coefficient data for  $\text{HO}_2$  are not available from Gordon *et al.* method. From a preliminary study, Gordon *et al.* method can be shown to be accurate as compared to the experimental data as for viscosity and thermal conductivity. As for  $\text{HO}_2$  mixture, the viscosity and thermal conductivity are calculated by Chapman-Enskog method (Chapman & Cowling 1991) and Eucken method (Poling, Prausnitz & O'Connell 2001), respectively. The Wilke method (Wilke 1950) and Wassiljewa method (Wassiljewa 1904) are used to estimate the multi-component gas viscosity and thermal conductivity based on the pure species values. The binary diffusion coefficients are evaluated using the Chapman-Enskog method (Chapman & Cowling 1991).

Particle tracking is employed to model the droplet motion. The governing equations for droplets are Newton's equation of motion, energy conservation equation, mass conservation equation and number density conservation equation.

$$m_i \frac{d\mathbf{u}_i}{dt} = \mathbf{f}_{\text{drag},i} + \mathbf{f}_{\text{pres},i} \quad (2.6)$$

$$m_i c_i \frac{dT_i}{dt} = q_{\text{conv},i} + q_{\text{evap},i} \quad (2.7)$$

$$\frac{dm_i}{dt} = \dot{m}_i \quad (2.8)$$

$$\frac{dn_i}{dt} = \dot{n}_i \quad (2.9)$$

Here,  $m_i$ ,  $c_i$  and  $\mathbf{f}_{\text{pres},i}$  are the WD mass, WD specific heat, and force due to the pressure gradient, respectively. The drag force  $\mathbf{f}_{\text{drag},i}$  is estimated using a model proposed by Ling *et al.* (2012). As the Biot number in this study is much less than unity, the intraparticle temperature gradient can be neglected. Additionally, the particle-specific heat is assumed to be constant. Droplet evaporation is estimated by the model proposed by Abramzon & Sirignano (1989). The convective heat flux is calculated using the Ranz–Marshall equation (Ranz & Marshall 1952). The droplet breakup occurs under the assumption that the droplet diameter decreases linearly during the breakup process (Chauvin *et al.* 2016). It is a phenomenological model based on the critical We number ( $We_c$ ) and the non-dimensional total breakup time which are modeled by Brodkey (1967) and Pilch & Erdman (1987), respectively. Even if the hydrodynamic model of Chauvin *et al.* (2016) differs from the present one, the numerical results can be shown to agree very well with each other. Comparison with experimental data of Chauvin *et al.* (2011) on shock interaction with a cloud of water droplets can be found in the Appendix B.

In most cases, the cellular structures can be retrieved with the use of the reactive Euler equations with a proper chemical mechanism. However, when the fuel comes to methane and propane-like based fuels, of which cellular structure can be classified as very highly irregular (Libouton *et al.* 1981), we cannot exclude turbulent burning of the unburnt pockets torn off by triple point collision (Radulescu 2018). Nevertheless, in our case of very weakly unstable detonation, the reactive Euler equations would be sufficient to retrieve the proper cellular structure. However as the initial pressure is very low (10 kPa) and there is few cells in the width of the channel (of which conditions have been chosen for resolution issues), we cannot exclude a priori the influence of the growth of the boundary layer on the detonation velocity. Computations of next sections have shown a posteriori that this is not the case (see Section 4.3) and that the detonation deficit comes from the presence of the water droplets. In addition, the additional water vapor from the evaporation of water droplets will mix with the gas phase, and the diffusion effect needs to be taken into account to estimate its influence on the reactivity of gaseous mixture.

The mean structure of 3D gaseous detonations has been addressed only recently (Taileb *et al.* 2018) and is still in its infancy, also due to its computational cost. However, 2D simulations have been shown to bring about the main qualitative features of gaseous detonations. This has driven the choice of a weakly unstable mixture, for which the third dimension will not bring quantitative modifications on the gas mean quantities. The only modification will be at the intersection of lines of triple points, which will influence very locally the droplet motion. However, this will not influence the mean quantities. Once again, different conclusions would have to be drawn for mildly or very unstable cases.

## 2.2. Numerical solvers

A classical time-splitting method is employed to couple the hydrodynamics with the detailed chemistry and the interphase exchanges. The spatial derivatives of the left-hand side of Eqs. (2.1)-(2.4) are discretized by fifth-order advection upstream splitting methods using pressure-based weight functions (AUSMPW+) improved by Kim, Kim & Rho (2001) based on modified weighted essentially non-oscillatory (MWENO-Z) (Hu, Wang & Chen 2016) and the diffusive terms by second-order central differential scheme. The time integration method for the convective and diffusion terms is the third-order total variation diminishing Runge-Kutta method (Gottlieb, Shu & Tadmor 2001), and

the multi-timescale method (Gou *et al.* 2010) is used for efficient time integration of the chemical source term.

The first-order symplectic Euler method (Cromer 1981; Tuley *et al.* 2010) is used for the integration of the Eq. (2.6) for droplets. For the time integration of Eqs. (2.7)-(2.9), the Euler explicit method is used.

The porosity is then calculated using the ratio of the total volume of droplets which locate inside the computational cell to the computational cell volume. For the summation of the total volume of droplets inside the computational cell, the particle centroid method is utilized (M. A. van der Hoef *et al.* 2008; Sun & Xiao 2015).

The gas phase quantities around the droplet to calculate the interphase exchanges are estimated by interpolating the surrounding three nearby Eulerian cell values by barycentric interpolation as in Shimura & Matsuo (2018).

The simulations used about 3.5 million cells, along with nine chemical species and 5 million Lagrangian parcels of particles with a typical cost of about  $\sim 10\,000$  CPU scalar hours. The wall is an adiabatic no-slip wall, and a transmissive boundary is applied to the left-hand side of the computational domain. The half reaction length ( $hrl$ ) in the present reaction model is  $1696\ \mu\text{m}$ . The minimum grid width is  $50\ \mu\text{m}$  and the resolution is then about 34 points per  $hrl$ . The Courant-Friedrichs-Lewy (CFL) number is fixed at 0.1 and the typical time step size is around  $10^{-9}$  s.

### 3. Problem statement

The physical configuration associated to the numerical simulations is depicted in Fig. 1. The premixed gas is chosen to be a stoichiometric  $\text{H}_2\text{-O}_2$  mixture diluted with 40%  $\text{N}_2$  at an initial pressure of 10 kPa and ambient temperature. Indeed, the post-shock non-dimensional activation energy ( $E_a/RT_{VN}$ ) for the premixed mixture in the present reaction model is 5.5. The premixed gas can then be classified as a weakly unstable mixture according to the stability analysis (Lee & Steward 1990; Austin 2003).

The width of the channel is 39 mm, which corresponds approximately to one cell and a half. Initially, the detonation is fully developed in the initial section of the computational domain, and then propagates toward the WD section. The WDs whose initial diameter and temperature are  $15.9\ \mu\text{m}$  and 300 K, respectively are uniformly distributed in the fresh gas. The apparent density of liquid is  $5.5\ \text{g/m}^3$ , of which mass loading is 7.45%.

The Reynolds average values are computed as follows

$$\bar{G} = \frac{1}{H} \int_0^H \left\{ \lim_{T \rightarrow \infty} \left( \frac{1}{T} \int_0^T G(x - x_s(y, t), y, t) dt \right) \right\} dy \quad (3.1)$$

In Eq. (3.1),  $H$  is the height of the channel,  $x_s(y, t)$  is the instantaneous position of the shock front, which is not straight due to cellular instabilities and  $T$  is the period of sampling. Then from the Reynolds averages, the Favre quantities can be obtained from the conservative variables  $\bar{\tau} = (\alpha\rho)_k \cdot / (\alpha\rho)_k$ ,  $k = \text{g or l}$ . This limit has been shown to exist since Radulescu *et al.* (2007) and more recent aforementioned references and that this mean steady state can be obtained for the subsonic reaction zone, which stands between the mean leading shock and sonic line. As they travel at the same velocities, the distance between them is the hydrodynamic thickness. However, this limit cannot describe the unsteady rarefaction waves, the Taylor-Zel'dovich wave, which takes place beyond.

From the comparison of the simulation results using the coarse grid in the Appendix C, the average quantities are converged with the present grid resolution. Moreover, Reynaud, Virot & Chinnayya (2017) have also shown that such resolution is sufficient to recover



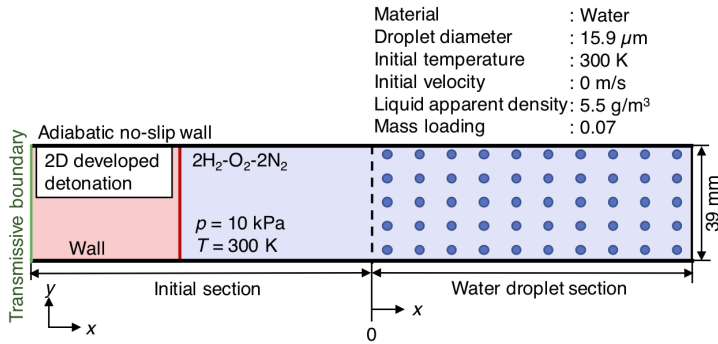


FIGURE 1. Computational initial conditions of two-phase detonation with dilute water spray

the gaseous averaged quantities. Therefore, conclusions on the mean structure are not called into question by the present numerical resolution.

The disturbances downstream of the last characteristic line do not influence the detonation front nor the propagation and the mean structure of gaseous detonation. Thus, the simulation is performed with a small computational domain which encompasses the mean leading shock and the mean sonic line. The computational domain is updated every time when the gaseous detonation approaches the right boundary, i.e. a new region is appended to the right of the computational domain and another is discarded on the opposite side. As the result of this procedure, the total number of droplets varies during the simulation by the recycling block method. Namely, the droplets are discarded once they leave the computational domain and the new droplets are added in the front of the detonation wave. The recycling block method (Reynaud, Virot & Chinnayya 2017; Sow, Chinnayya & Hadjadj 2019; Mi, Timofeev, Higgins 2017; Mi *et al.* 2017) is used to reduce the computational cost with a relatively smaller computational domain and allows the detonation to run a long distance enough to compute mean and statistical values. Details can be found in Sow, Chinnayya & Hadjadj (2019).

The length of the computational domain with minimum grid size is set to 120 mm in the present study. The length of the front detonation propagation in the computations which are shown in this study is 900 mm. Then in order to get the averaged values, the instantaneous 2D flow fields are saved each time the detonation front has propagated 1 mm, from 300 mm to 900 mm after the first contact with WDs section. Afterwards, the six hundred one-dimensional profiles can be obtained, from which we get finally the Favre mean one-dimensional profiles.

For the simulation of gaseous detonation, a finer mesh is desirable to capture the flow field details. However, the mesh size should be larger than the droplet size in the present numerical method. Therefore, there is a trade-off between mesh resolution for gaseous detonation and droplets. The low pressure of the initial mixture enables us to have a large half-reaction length and a mesh resolution of 50  $\mu\text{m}$ , which is larger than the size of 15.9  $\mu\text{m}$  of the droplets. This mesh resolution corresponds to about 34 points per half reaction length, which is enough to capture the detonation structures of this weakly unstable mixture.

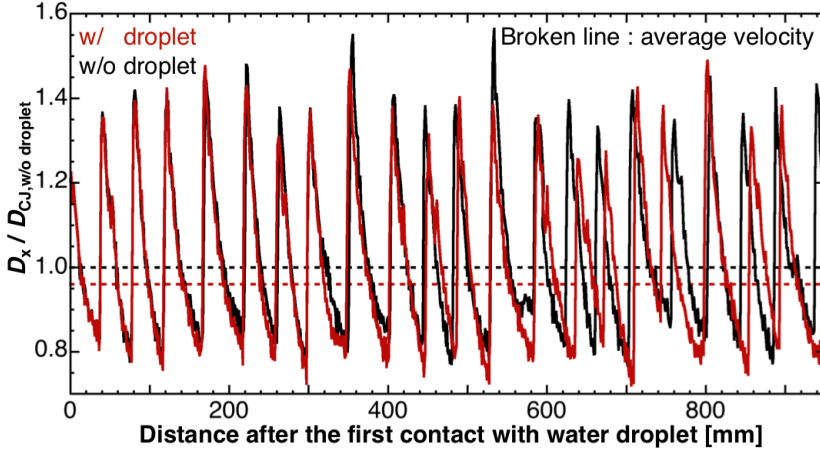


FIGURE 2. Normalized propagation velocity on the bottom wall

## 4. Results and discussions

### 4.1. Propagation velocity

To capture the propagation behavior and front structure globally, the propagation velocity is presented in this subsection. The propagation velocity on the bottom wall is shown in Fig. 2. The propagation velocity with WDs starts to change from the profile without WDs after the first contact with WDs. Both peak and minimum velocities become lower due to the interaction with WDs. To analyze the propagation velocity, the Probability Density Function (pdf) for the detonation velocity is shown in Fig. 3. Without WDs, the mean detonation velocity ( $D_{CJ,w/o\ droplet} = 2111$  m/s) agrees well with the theoretical dry case (CEA calculation (McBride & Gordon 1996)). With WDs, the mean detonation velocity shows a decrease of 3.8% as compared to the previous dry case. The instantaneous propagation velocity ranges from 0.8 to 1.6 CJ velocity and the pdf distribution is skewed toward the sub-CJ velocity. The peak value of the distribution is 0.9 in the present study. The overall shape of pdf in Fig. 3 is similar between both cases and the same power-law dependence is observed (Radulescu *et al.* 2007). However, the percentage below dry CJ speed increases from around 50% (without WDs) to 60% by the addition of WDs.

### 4.2. Global features

This subsection is devoted to the study of the instantaneous features of the flow fields in order to address the differences, which come from the presence of the liquid dispersed phase. Figure 4 depicts the gas phase instantaneous 2D flow fields without WDs. The different quantities are (a) pressure, (b) gas density, (c) gas temperature, (d) gas velocity in  $x$ -direction in mean shock frame, (e) Mach number in mean shock frame, (f) gas velocity in  $y$ -direction, (g) mass fraction of  $H_2O$ , (h) Q criterion, (i) maximum pressure, respectively. The maximum pressure history in Fig. 4(i) corresponds to soot foils in experiments. The number of cells inside the channel is 1.5. The cellular structure is regular, with a characteristic saw-tooth shape of the interface between the inert and burned gases and no large fresh pockets of gas downstream can be seen (Figs. 4(c) and 4(g)). The boundary layer growth can also be observed near the wall behind the shock wave (Figs. 4(d), (e) and (h)). But it is too thin to affect the propagation velocity as the

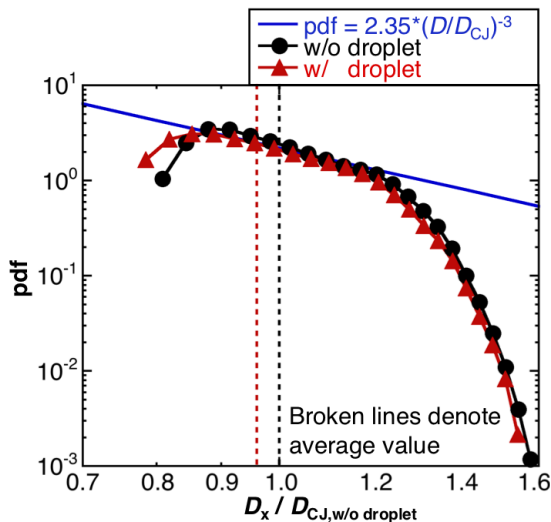


FIGURE 3. pdf of detonation propagation velocity

ideal theoretical detonation velocity is retrieved. The vapor water is in thermochemical equilibrium state far from the leading shock waves in the absence of WDs (Fig. 4(g)).

Figure 5 depicts the gas phase instantaneous 2D flow fields for gaseous detonation with WDs. The quantities are (a) pressure, (b) gas density, (c) gas temperature, (d) gas  $x$ -velocity in mean shock frame, (e) Mach number in mean shock frame based on the gas sound speed, (f) gas  $y$ -velocity, (g)  $H_2O$  mass fraction, (h)  $Q$  criterion, (i) maximum pressure, respectively. The instantaneous 2D flow fields for interphase exchange by WDs are shown in Fig. 6. The different quantities are (a) evaporation rate, (b) momentum transfer rate in  $x$ -direction, (c) momentum transfer in  $y$ -direction, (d) energy transfer rate, respectively. Furthermore, Fig. 7 shows the droplet instantaneous 2D flow fields for (a) droplet volume fraction, (b) number density, (c) droplet mass ratio, (d) droplet diameter, (e) droplet  $x$ -velocity, (f) droplet  $y$ -velocity, (g) droplet temperature, (h) particle Mach number  $|u_g - u_1|/c_g$ , (i) Weber number  $\rho_g |u_g - u_1|^2 d/\sigma$ , (j) total breakup time, respectively. The Figs. 6(a-d) and 7(a) correspond to Eulerian fields whereas the Figs. 7(b-j) represent Lagrangian data and the white color in Figs. 7(b-j) means that there is no droplet.

The overall cellular detonation structure looks similar to what would be the detonation without WDs, still constituted of incident shocks, Mach stems and transverse waves. Indeed, the cellular structure with WDs does not change drastically even if the propagation velocity decreases by 3.8% compared with the dry CJ velocity (see Figs. 4(i) and 5(i)). However, closer inspection reveals differences. This lower propagation velocity will induce a lower post-shock gas pressure. The pressure in the wet case in Fig. 5(a) will then overtake that of the dry case in Fig. 4(a) as the two-phase interactions take place. The same behavior in Figs. 4(b) and 5(b) can be seen as for the density, as water vapor from the liquid phase evaporation is released in the gas phase from evaporation (Fig. 6(a)). Moreover, from temperature and water vapor flow fields comparison (see Figs. 4(c,g) and 5(c,g)), the lower detonation velocity can be seen to induce a greater induction length, behind the incident shocks. However, on the contrary of what would be expected, the flow fields of the gas velocity components and its gradient in Figs. 4(d,e,f,h) and 5(d,e,f,h) exhibit less complicated structures and vortices are even suppressed by the WDs presence (Figs. 4(h) and 5(h)).

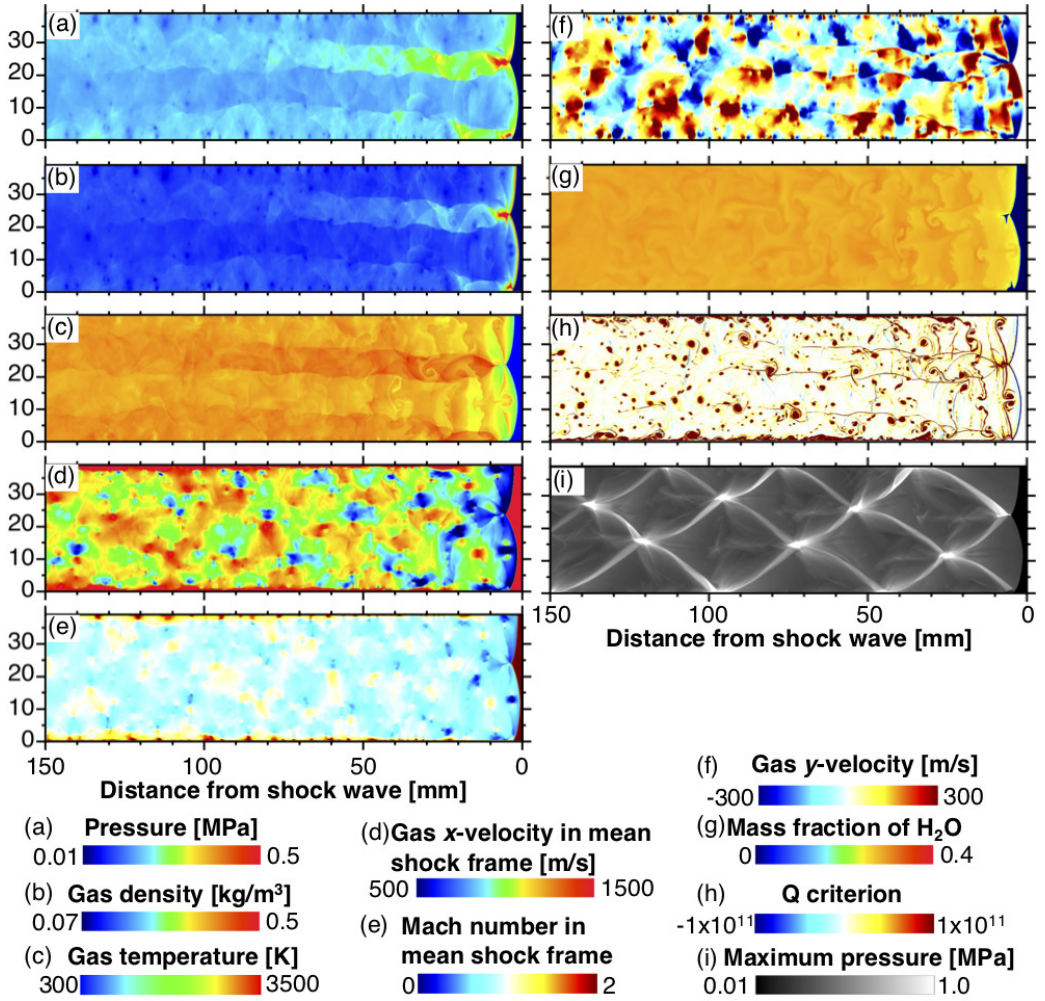


FIGURE 4. 2D flow fields for gas phase without water droplets. (a) Pressure, (b) Gas density, (c) Gas temperature, (d) Gas  $x$ -velocity in mean shock frame, (e) Mach number in mean shock frame, (f) Gas  $y$ -velocity, (g) Mass fraction of  $\text{H}_2\text{O}$ , (h)  $Q$  criterion, (i) Maximum pressure

The flow field for droplet volume fraction which is uniformly distributed initially shows preferential concentration (Fig. 7(a)), of which reason is not completely known yet, and jets from triple point collision and shear layers should play probably a central role. Then further from the leading shock, the liquid volume fraction decreases due to the evaporation process. Its rate is highest in the higher liquid concentration zones. The water vapor content is then increased, compared to the dry case (Figs. 4(g) and 5(g)).

In the first 15-20 mm behind the leading shock, the droplet velocity remains relatively low (Figs. 7(e) and 7(f)), inducing the highest momentum transfer rates (Figs. 6(b) and 6(c)). The droplet motion seems mainly driven by the high speed forward and backward jets generated by triple point and transverse wave collisions. Moreover, the droplet trajectory depends on its inertia and therefore on its diameter, which decreases due to two processes: breakup and evaporation. The former takes place within a narrower zone in the first 10 mm (Figs. 7(j) and 7(b)), the latter then taking over (Fig. 7(c)). The particle Mach number (Fig. 7(h)) and the Weber number (Fig. 7(i)) decrease accordingly

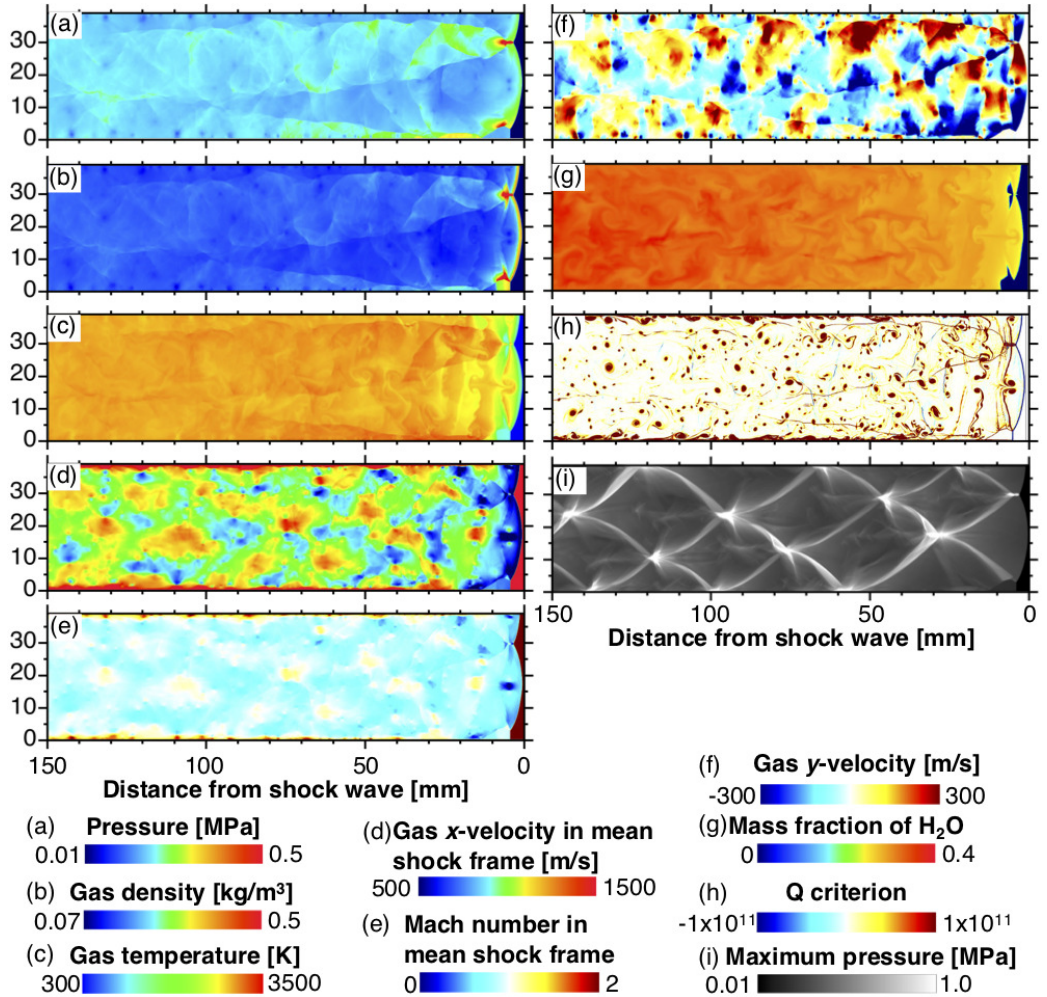


FIGURE 5. 2D flow fields for gas phase with water droplets. (a) Pressure, (b) Gas density, (c) Gas temperature, (d) Gas  $x$ -velocity in mean shock frame, (e) Mach number in mean shock frame, (f) Gas  $y$ -velocity, (g) Mass fraction of H<sub>2</sub>O, (h) Q criterion, (i) Maximum pressure

due to the decrease of both diameter and relative velocity. The WDs are then more likely to follow the gas. Nevertheless, they seem more likely to lie near the shear layers, which are torn off by the triple point collision and convected downstream.

The WDs accelerate after the shock wave passage due to pressure and drag forces and approach velocity equilibrium with gas in the horizontal direction (Fig. 7(e)). However, the WD velocity in  $y$ -direction fluctuates due to the transverse waves and velocity equilibrium in the  $y$ -direction is not achieved (Fig. 7(f)). Indeed, the transverse waves which pertain long downstream of the shock lead to rapid and sudden changes of  $y$ -gas velocity (Figs. 5(f) and 7(f)), inducing  $y$ -momentum transfer (Fig. 6(c)).

As for temperatures, the droplet temperature reaches very rapidly the saturation temperature (Fig. 7(g)), being the fastest relaxation process (Guha 1992), before the beginning of evaporation (Fig. 6(a)). A temperature disequilibrium between the gas and liquid phases remains during all the detonation process.

After the shock passage, the flow becomes subsonic, and then as the gas velocity is

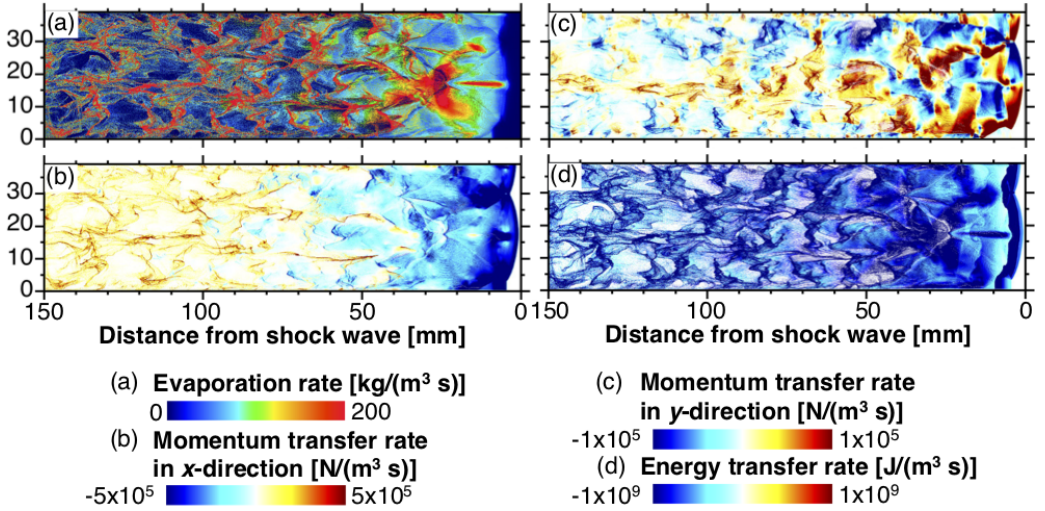


FIGURE 6. 2D flow fields for interphase exchange by water droplets. (a) Evaporation rate, (b) Momentum transfer rate in  $x$ -direction, (c) Momentum transfer rate in  $y$ -direction, (d) Energy transfer rate

accelerated by burned gas expansion in both cases in Figs. 4(e) and 5(e), the flow becomes gradually supersonic. However, some supersonic pockets appear due to the definition of the Mach number, which is based on the mean detonation velocity, whereas a more proper definition should rely on limiting characteristic surfaces (see Kasimov & Stewart 2004; Stewart & Kasimov 2005). In addition, the gas total energy decreases constantly along with the interaction with WDs behind the shock wave (Fig. 6(d)). As the result of momentum and energy transfer, the gas  $x$ -velocity in the shock fixed frame is lower (Fig. 5(d)). The high relative velocity in  $x$ -direction immediately downstream of the leading shock implies the particle Mach number being over one and the flow around the WDs being supersonic. Then as velocity equilibrium in the  $x$ -direction is approached, the particle Mach number becomes subsonic again (Fig. 7(h)).

Even if velocity equilibrium is achieved only in one direction, the Weber number is greater than the critical Weber number only at the vicinity of the leading shock (Fig. 7(i)). As can also be seen in Fig. 7(j), the order of magnitude of the total breakup time is around  $5 \mu\text{s}$ . Breakup generated a lot of smaller daughter droplets. This process occurs mainly at the vicinity of triple point and transverse wave collisions (Fig. 7(b)). The evaporation of WDs is enhanced by the smaller droplet diameter and the mass of the droplet decreases as the time passes (Fig. 7(c)).

#### 4.3. Mean structure for gaseous phase

In order to analyze quantitatively the differences between the dry and wet cases, the Favre average (Favre 1965) in time and space in the frame of the instantaneous detonation motion is obtained from the simulations, following previous studies (Radulescu *et al.* 2007; Lee & Radulescu 2005; Maxwell *et al.* 2017; Reynaud, Virost & Chinnayya 2017; Sow, Chinnayya & Hadjadj 2014; Sow, Chinnayya & Hadjadj 2015; Sow, Chinnayya & Hadjadj 2019; Mi, Timofeev & Higgins 2017; Mi *et al.* 2017) and Eq. (3.1). In order to deal with multiphase features, gas phase quantities are weighted by the gas apparent density  $(\alpha\rho)_g$  and the liquid quantities by  $(1-\alpha_g)\rho_l$ . The one-dimensional Favre averaged profiles for gas phase are shown in Fig. 8, which shows (a) pressure, (b) gas density, (c) gas temperature, (d) estimation of Mach number in the mean shock frame, (e) gas  $x$ -

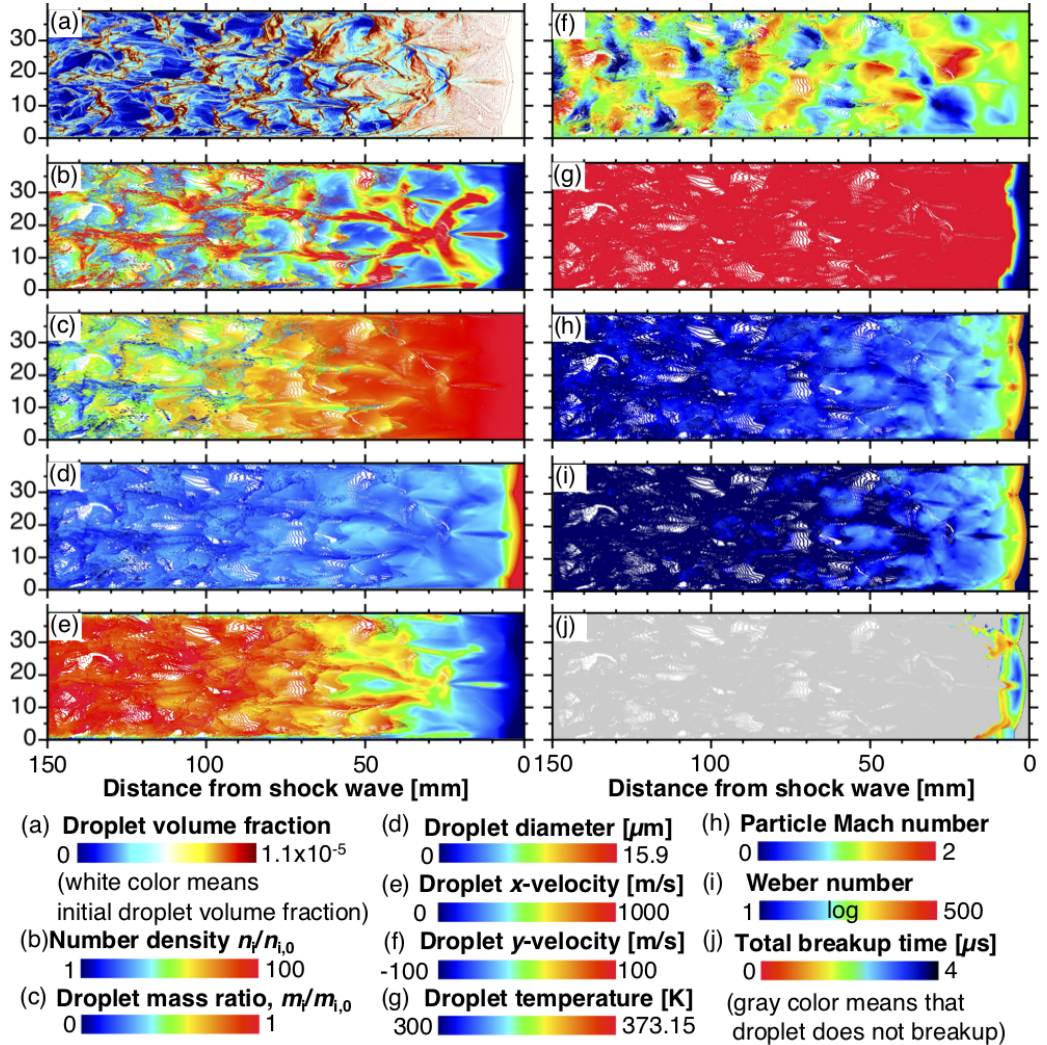


FIGURE 7. 2D flow fields for water droplets. (a) Droplet volume fraction, (b) Number density, (c) Droplet mass ratio, (d) Droplet diameter, (e) Droplet  $x$ -velocity, (f) Droplet  $y$ -velocity, (g) Droplet temperature, (h) Particle Mach number, (i) Weber number, (j) Total breakup time

velocity in the mean shock frame, (f) sound speed, (g)  $\text{H}_2$ , (h)  $\text{H}_2\text{O}$  (i) OH mass fraction, (j) thermicity, respectively. The horizontal axis in Fig. 8 is normalized by the  $h_{rl}$ .

The behavior of the mean pressure and gas density and their differences (Figs. 8(a)(b)) can clearly be visualized. The lower detonation velocity of the wet case induces a lower post-shock pressure. The density at the von Neumann (vN) in Fig. 8(b) is about the same. However, further from the shock, the decrease of the pressure is tampered and the gas density is also increased, due to the different relaxation processes (Guha 1992; Rudinger 1964). In addition, the gaseous velocity decreased as would be expected from the presence of the liquid dilute phase (Fig. 8(e)). The sound speed in two-phase mixture  $c_{\text{two}}$  can be evaluated by following formula (Brennen 2005) under the assumption that the velocities

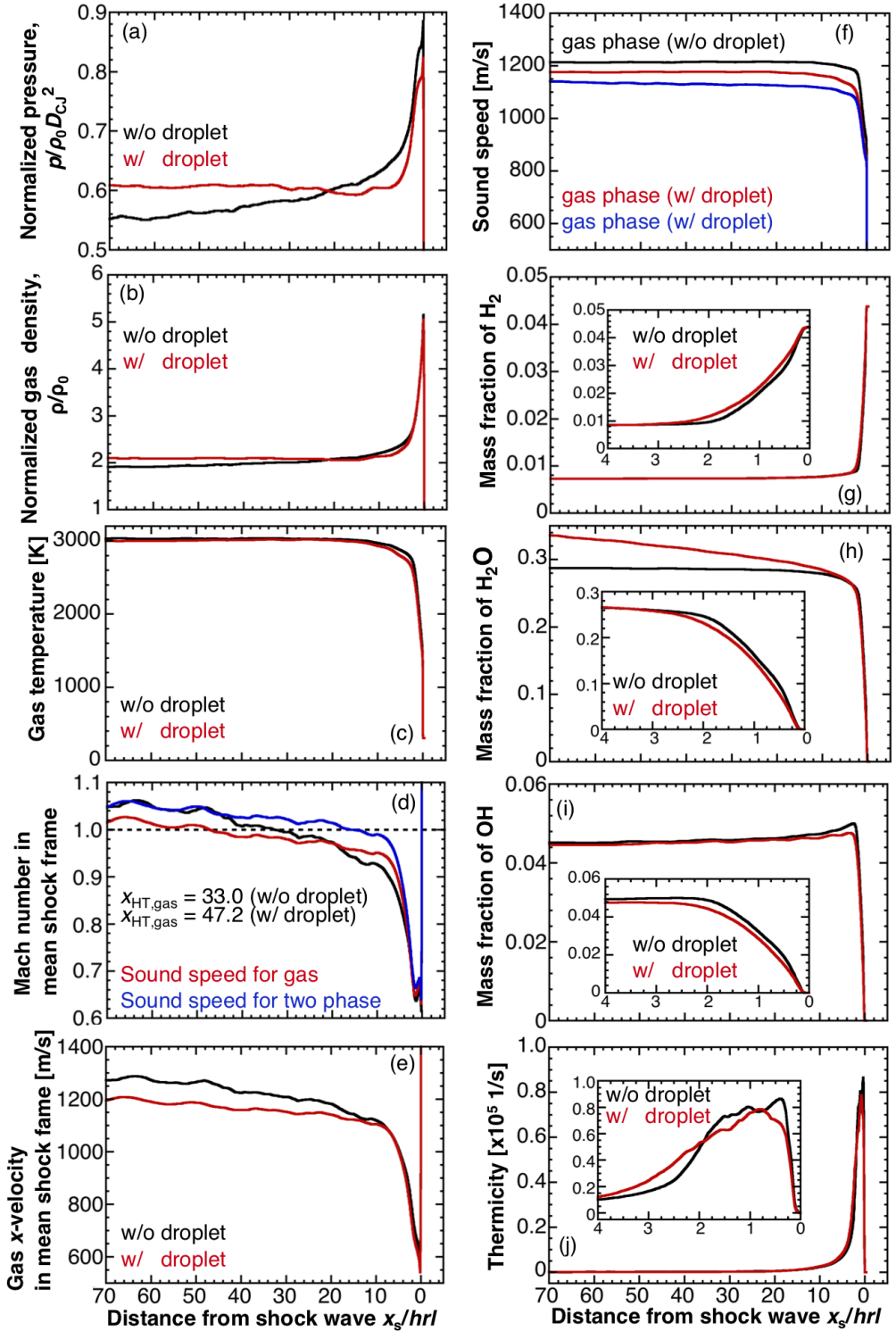


FIGURE 8. Favre averaged profiles for gas phase. (a) Pressure, (b) Gas density, (c) Gas temperature, (d) Mach number in mean shock frame, (e) Gas  $x$ -velocity in mean shock frame, (f) Sound speed, (g) Mass fraction of  $H_2$ , (h) Mass fraction of  $H_2O$ , (i) Mass fraction of OH, (j) Thermicity



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of both phases are in equilibrium.

$$c_{\text{two}} = \left( \frac{\gamma_g p_g}{\alpha_g ((1 - \alpha_g) \rho_l + \alpha_g \rho_g)} \right)^{1/2} \quad (4.1)$$

Here  $\gamma_g$  and  $\rho_l$  are specific heat ratio of gas and liquid density, respectively. The estimation of the sound speed for two-phase mixture defined by Eq. (4.1) is valid under thermal disequilibrium and is lower than the sound speed in gas phase all the more so as the gas volume fraction  $\alpha_g$  decreases. That explains why the Mach number based on Eq. (4.1) is greater than the gaseous Mach number in Fig. 8(d). However, the sound speed in Eq. (4.1) holds for two-phase mixtures in velocity equilibrium, which does not stand in our case. Thus, it is expected that the group velocity of the pressure waves should be between those two. We have seen in previous sub-section 4.2 that the level of fluctuations is lowered with the WD presence. However, the hydrodynamic thickness is further delayed. The hydrodynamic thickness (HT) without WDs and with WDs based on sound speed for gas  $x_{\text{HT,gas}}$  are 33.0 and 47.2 *hrl*, respectively. This could be due to the gaseous phase being continuously cooled by the liquid phase, due to evaporation.

In the case with WDs, evaporation produces water vapor so that the amount of  $\text{H}_2\text{O}$  is higher than that by the only combustion of hydrogen-oxygen mixture as shown in Fig. 8(h). This figure also shows that evaporation mainly takes place further downstream from the shock. Moreover, the amount of  $\text{H}_2$  is the same (Fig. 8(g)) and the profiles of mass fraction of OH is similar between both cases (Fig. 8(i)), even if there is release of water vapor within the flow, indicating a strong interaction with the chemical mechanism.

The profile of the thermicity in Fig. 8(j), which is computed from the mean values obtained by the averaging process becomes thicker. However, the peak which is little lower remains approximately at the same position. In the present study, the induction length is estimated from the distance from the shock to the position of peak thermicity maximum. The estimation of the induction length  $x_{\text{ind,thermicity}}$  is 0.4 *hrl* in the dry case and 0.7 *hrl* in the wet case, respectively. Another method recommended by Austin and Shepherd (2003) to estimate the induction length  $x_{\text{ind,OH}}$  is from the position of the peak of OH. In that case, this estimation of  $x_{\text{ind,OH}}$  is 2.6 and 3.4 *hrl* for the dry and wet case, respectively. After close inspection, two nearby peaks can be inferred from the thermicity profiles. The increase in the induction length by the first peak is in line with the 3.8% decrease in the detonation velocity. However, the cell size which is roughly proportional to the induction length does not change much. As a conclusion, the estimation of the induction length in this study will be considered to be 0.4 ~ 3.4 *hrl*. Moreover, the reaction length was at first estimated as the distance from the shock to the position where the thermicity is 1% of the maximum thermicity  $x_{\text{reac,1\%}}$  and then from the ratio of the peak thermicity maximum to the velocity at the CJ state  $x_{\text{reac,max}}$  as suggested by Radulescu (2003) and Ng *et al.* (2005).

$$x_{\text{reac,max}} = u_{\text{CJ}} / \dot{\sigma}_{\text{max}} \quad (4.2)$$

Here,  $u_{\text{CJ}}$  is the gas velocity at the CJ plane and  $\dot{\sigma}_{\text{max}}$  is the maximum value of thermicity. For the dry case, both estimates give similar results 13.3 and 15.7 *hrl*, whereas for the wet case they give 13.6 and 15.9 *hrl*, respectively. When the two-phase sound speed is used, the same value of 13.0 *hrl* is obtained. As a result, the characteristic induction length  $x_{\text{ind}}$  increases with WDs presence, whereas the reaction length  $x_{\text{reac}}$  remains almost the same.

In order to quantify the growth of the boundary layer, the displacement thickness and momentum thickness are depicted in Fig. 9 based on the Favre averaged 2D flow fields. The boundary layer develops downstream of the leading front. There are some

	w/o droplet	w/ droplet
$x_{\text{ind,themicity}}$	0.4	0.7
$x_{\text{ind,OH}}$	2.6	3.4
$x_{\text{reac,1\%}}$	15.7	15.9
$x_{\text{reac,max}}$	13.3	13.6 (gas sound speed based)
	-	13.0 (two-phase sound speed based)
$x_{\text{HT,gas}}$	33.0	47.2

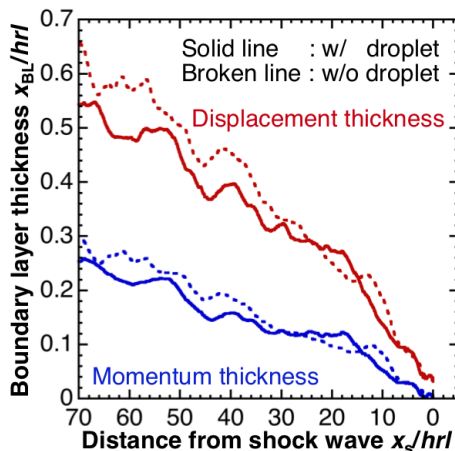
TABLE 1. Characteristic lengths for gaseous detonation (normalized by  $hrl$ )

FIGURE 9. Boundary layer growth

oscillations which remain in the profiles due to continuous impingement of transverse waves. The boundary layer in the case without WDs seems thicker than that with WDs, the reason of which is beyond the scope of the present study even if particularly relevant for practical applications. In both cases, the boundary layer thickness remains small compared to the channel width so that the propagation velocity is not affected by the boundary layer growth (see Section 4.1).

The different characteristic lengths for gaseous detonation in the present study are summarized in the Table 1.

#### 4.4. Droplet behavior

In this section, the behavior of WDs is quantitatively analyzed through Favre averaging process. The WDs Lagrangian data are at first projected on the Eulerian grid and then the same averaging process as in the previous section is applied. Figure 10 shows the Favre averaged one-dimensional profiles for water droplets, (a) droplet volume fraction, (b) droplet diameter, (c) Weber number, (d) particle Reynolds number and particle Mach number, (e) force acting on WDs, (f) the characteristic time for evaporation and breakup, (g) square of droplet diameter, (h) number density, (i) droplet mass ratio, respectively. The characteristic time for breakup is taken as the total breakup time, and characteristic time for evaporation  $\tau_{\text{evap}}$  is defined by the following equation in this study.

$$\tau_{\text{evap}} = m/\dot{m} \quad (4.3)$$

Here,  $m$  and  $\dot{m}$  are the mass of WDs and the evaporation rate of WDs, respectively. To

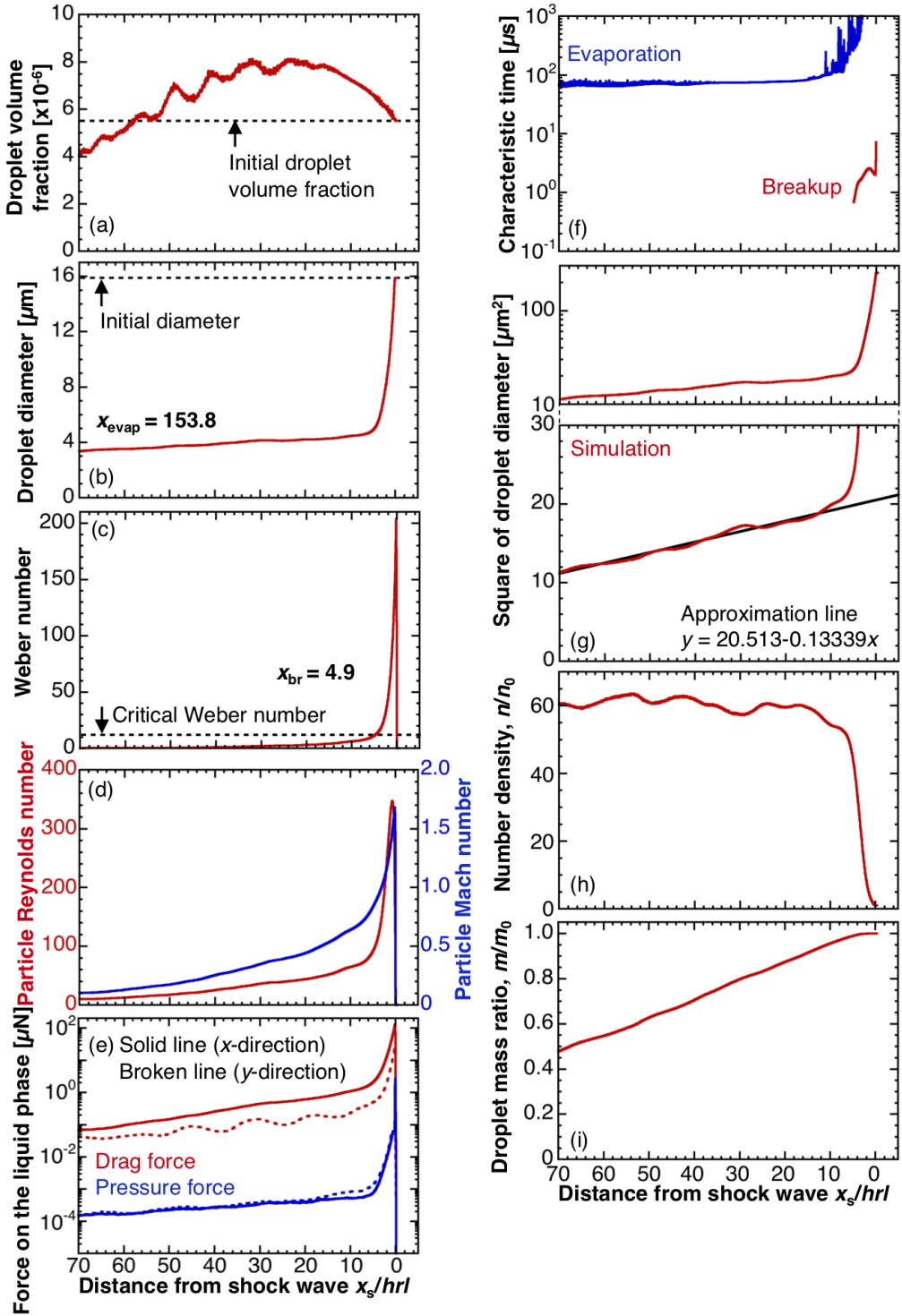


FIGURE 10. Favre averaged profiles for water droplets. (a) Droplet volume fraction, (b) Droplet diameter, (c) Weber number, (d) Particle Reynolds number and particle Mach number, (e) Force acting on droplet, (f) Characteristic times for evaporation and breakup, (g) Square of droplet diameter, (h) Number density, (i) Droplet mass ratio

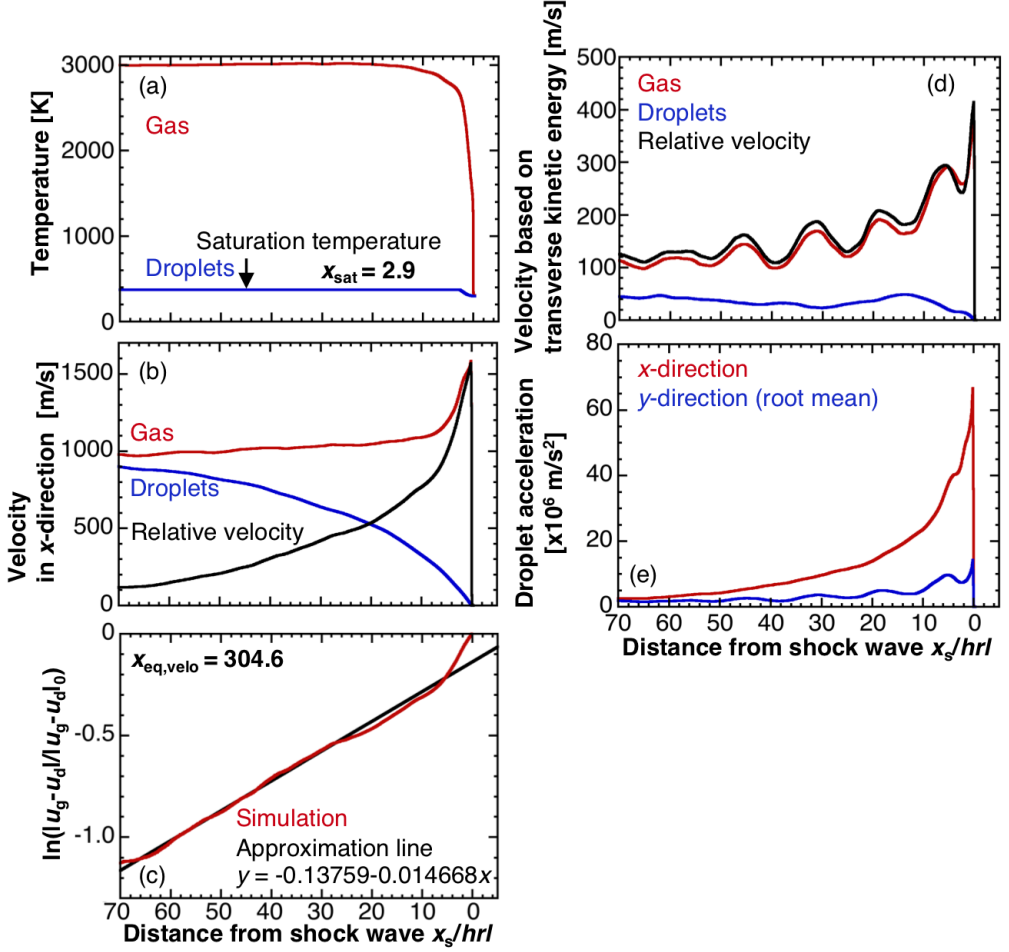


FIGURE 11. Comparison between gas and droplets quantities. (a) Temperature, (b)  $x$ -velocities, (c) Normalized relative  $x$ -velocity, (d) velocity based on transverse kinetic energy, (e) Droplet acceleration

indicate the velocity and temperature equilibration between gas and WDs, Fig. 11 shows (a) temperature, (b)  $x$ -velocity, (c) slope for relative  $x$ -velocity, (d)  $y$ -velocity of gas and droplets and relative  $y$ -velocity, (e) acceleration of WDs, respectively.

From the Fig. 10(a), the liquid volume fraction increases at first due to drag between phases. Then, the droplet mass decreases (Fig. 10(i)), indicating that the evaporation implies the decrease of the volume fraction of WDs, after the droplets have reached the saturation temperature (Fig. 11(a)).

The WDs with an initial uniform diameter of  $15.9 \mu\text{m}$  sharply decreases to about  $5 \mu\text{m}$  after the leading shock wave passage and then gradually decreases to around  $3 \mu\text{m}$  (Fig. 10(b)). From Fig. 10(f), the breakup time is much shorter than that of evaporation immediately behind the shock where the droplet diameter and the relative velocity are the greatest, highlighting the dominant role of the breakup. The end of breakup can be seen in Figs. 10(c)(f). As a result of breakup, a single parent droplet gives birth to about 60 daughter droplets (Fig. 10(h)). Indeed, the Weber number which is highest after the shock then falls below the critical Weber number (around 12), which comes from the decrease of the droplet diameter towards its equilibrium value, but also due to the decrease of

relative velocity. In this study, the characteristic length for breakup  $x_{br}$  is defined as the distance from the shock wave to the position where the Weber number becomes  $We_c$ . Under the present calculation conditions, the characteristic length for breakup is  $4.9 hrl$  from Fig. 10(c). The breakup completes after the induction zone ( $x_{ind,thermicity} = 0.7 hrl$ ).

As shown in Fig. 10(i), the evaporation of WDs is not completed within the computational domain. Indeed, the droplet mass ratio based on the initial mass constantly decreases and becomes 0.47 at  $70 hrl$  from the mean shock position. After the completion of breakup, the square of the droplet diameter can be seen to vary linearly with the distance to the shock (Fig. 10(g)), which is reminiscent of the evaporation  $d^2$  law and which emphasizes the fact that the droplet varies only by evaporation in this flow region. Therefore, the characteristic length for evaporation  $x_{evap}$  is the distance for WDs to finish evaporation and is evaluated from the linear approximation after the breakup, i.e., the region between 10 to  $70 hrl$  from the shock wave (Fig. 10(g)). This evaporation characteristic length is estimated to be  $153.8 hrl$ .

The gas and WDs temperature are shown in Fig. 11(a). The gas temperature increases by exothermic chemical reactions. The temperature of WDs also increases due to the convective heat transfer with gas phase and then reaches the saturation temperature at the distance of  $2.9 hrl$ , of which will be shown to be the fastest of all the relaxation processes. The temperature of WDs does not equilibrate with the gas temperature, which means that temperature equilibrium is not achieved. The characteristic length for temperature equilibrium  $x_{sat}$  is defined as the distance from the shock wave to the position where the WDs reaches the saturation temperature, and is estimated as  $2.9 hrl$ .

The gas phase in the laboratory frame gets accelerated by the shock wave and then decreases due to the expansion of burned gas (Fig. 11(b)). The WDs are accelerated due to quasi-steady drag and pressure forces. Due to these momentum transfers, the velocity of the droplet increases and that of the gas decreases to the equilibrium value. As a result, the relative velocity in  $x$ -direction between the gas and WDs is maximum immediately after the shock wave and gradually decreases to one tenth of the maximum at the distance of  $70 hrl$  from the mean shock position. The ratio of the relative  $x$ -velocity to its initial value at the vN state is plotted as a function of distance in Fig. 11(c). After some transients, the slope is constant despite the change in the diameter due to evaporation, breakup and the pressure gradient, from which a time constant can be deduced. The characteristic length for velocity equilibrium in  $x$ -direction  $x_{eq,velo}$  is defined as the distance from the shock wave to the position where the relative velocity decreases to 1% of its maximum. Under the present conditions, the characteristic length for the velocity equilibrium in  $x$ -direction is estimated as  $304.6 hrl$ .

In order to obtain the spanwise contribution, the gas velocity in the  $y$ -direction is estimated as follows:  $\tilde{v}_g = (\alpha_g \rho_g v_g^2 / \tilde{\alpha}_g \rho_g)^{1/2}$ . The same procedure is for the liquid spanwise velocity. The following is used for relative spanwise velocity  $\sqrt{(v_g - v_l)^2}$ . The gas spanwise contribution is maximum at the shock and then decreases (Fig. 11(d)). However, the fluctuations of gas velocity in  $y$ -direction remain large and the  $y$ -velocities do not seem to approach equilibrium (Fig. 11(d)).

The particle Reynolds number and the particle Mach number are also shown in Fig. 10(d). They have a maximum at the shock and then gradually decrease. The peak value of the particle Mach number is relatively high, with a value of 1.7 due to the high relative post-shock velocity. Thus, compressibility effects may have a large influence on the flow field around the WDs. As for the particle Reynolds number, the peak value immediately after the shock wave is relatively low, about 300 because the diameter of

	w/ droplet
$x_{\text{sat}}$	2.9
$x_{\text{br}}$	4.9
$x_{\text{eq,velo}}$	304.6
$x_{\text{evap}}$	153.8

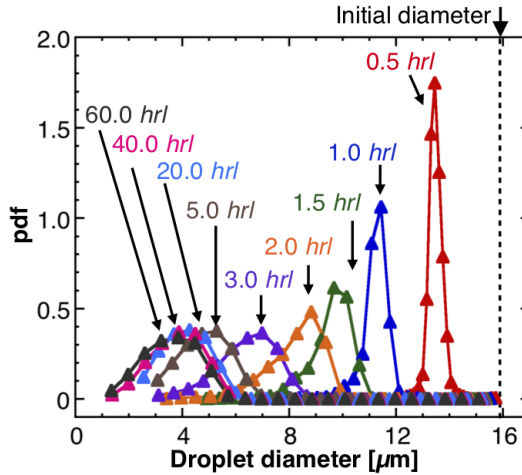
 TABLE 2. Characteristic lengths for liquid dispersed phase (normalized by  $hrl$ )


FIGURE 12. Probability density function for droplet diameter as a function of the diameter for several distances from the shock

WDs is small of the order of  $\mu\text{m}$  and the initial pressure is rather low in the present study. The particle Reynolds number rapidly decreases to about 60 due to the rapid decrease in diameter and relative velocity, and is about 20 at the end of the computational domain.

Both the quasi-steady drag and pressure drag are also maximum after the shock, and the force acting on the WDs becomes 2,3 order less at the end of the computational domain (Fig. 10(e)). The magnitude of the quasi-steady drag is determined by the relative velocity and the diameter. Again, lower diameter and relative velocity further from the front induce the decrease of these two contributions in the momentum transfer. Their  $x$  and  $y$ -components are comparable. In addition, pressure drag is much smaller than quasi-steady drag by three orders of magnitude (Fig. 10(e)). The acceleration of WDs in both  $x$  and  $y$ -directions become maximum at the detonation front and smaller as the WDs move from the shock wave (Fig. 11(e)). Since the quasi-steady drag which is the dominant force acting on the WDs is larger in  $x$ -direction than in  $y$ -direction, the acceleration of the WDs in  $x$ -direction is larger than that in  $y$ -direction from Fig. 11(e). The acceleration of the WDs is proportional to the cube of the reciprocal of the diameter and the force acting on the WDs. The diameter is about one fourth of the initial droplet diameter at the end of the computational domain (Fig. 10(b)) and the force acting on the WDs is smaller by two or three orders of the magnitude compared to its maximum value (Fig. 10(e)). Therefore, the acceleration decreases, mainly due to the decrease of the momentum transfer between phases, which come from the decrease of the diameter and the drag.

The different characteristic lengths for WDs in the present study are summarized in Table. 2.

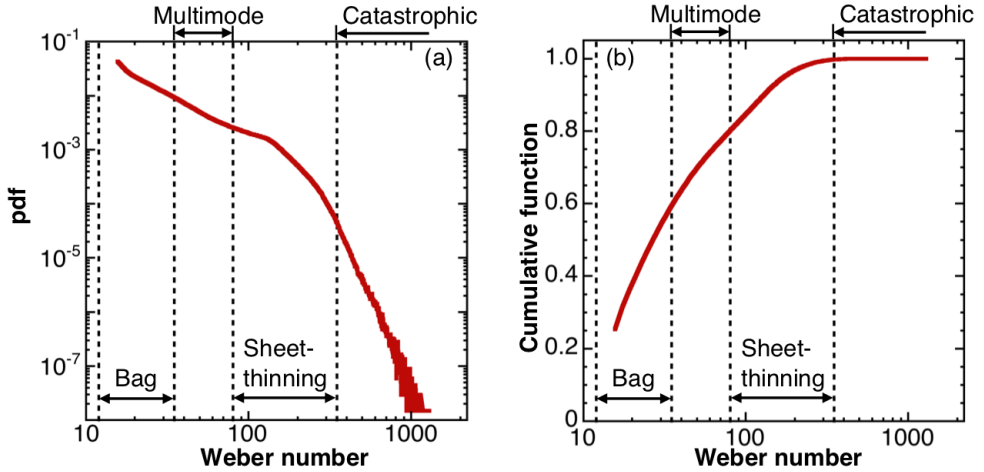


FIGURE 13. Breakup regime. (a) Probability density function for Weber number exceeding the critical Weber number, (b) Cumulative function for Weber number exceeding the critical Weber number

In the Favre averaged one-dimensional profile on the droplet diameter shown in Fig. 10(b), the polydispersity in diameter observed in Fig. 7(d) and the process of breakup cannot be evaluated. Figure 12 shows the pdf on the diameter as a function of the diameter for several distances from the shock. Indeed, the process of breakup is not uniform downstream of the leading detonation front. The latter is composed of incident shocks, Mach stems and transverse waves, all of which have different intensities. Thus, even though the initial droplet diameter is uniform, the polydisperse spray is the result of the interaction of breakup with the detonation cellular instabilities. The pdf of droplets is shown in Fig. 12 for the positions 0.5, 1.0, 1.5, 2.0, 3.0, 5.0, 20.0, 40.0 and 60.0 *hrl*. After the breakup process, which is completed at 4.9 *hrl* (Fig. 10(c)), the shape of pdf is similar and the diameter only gradually decreases by evaporation of WDs, the influence of the cellular instabilities being reduced.

Figure 13 represents the pdf and the cumulative function distribution for the Weber number exceeding the critical Weber number to show the breakup mode which the WDs experience in the present study. According to the review by Guildenbecher, Lopez-Rivera & Sojka (2009), the different breakup scenarios are bag, multimode, sheet-thinning and catastrophic breakup. Although the maximum Weber number is high up to 1200, the percentage of bag, multimode, sheet-thinning and catastrophic breakup is about 60%, 20%, 20% and 0.3% from Fig. 13(b) for the present calculation conditions. The breakup causes a decrease in diameter but also a polydisperse spray, highlighting the important influence of the breakup of the droplet during its course in the detonation cell, the leading shock continuously decelerating along with further impingements from transverse shock waves.

#### 4.5. Interphase interactions and Master equation

The interphase exchanges rates which are the right-hand side terms of Eqs. (2.1)-(2.3) are evaluated in Fig. 14. Figure 14(a) confirms that evaporation is promoted by breakup, as the droplet size is greatly decreased. Indeed, only 1% of WDs can be estimated to be evaporated during this first phase. Then, evaporation rate is rather constant, with a slight peak, the temperature difference between phases that is not relaxed, being the driven force.

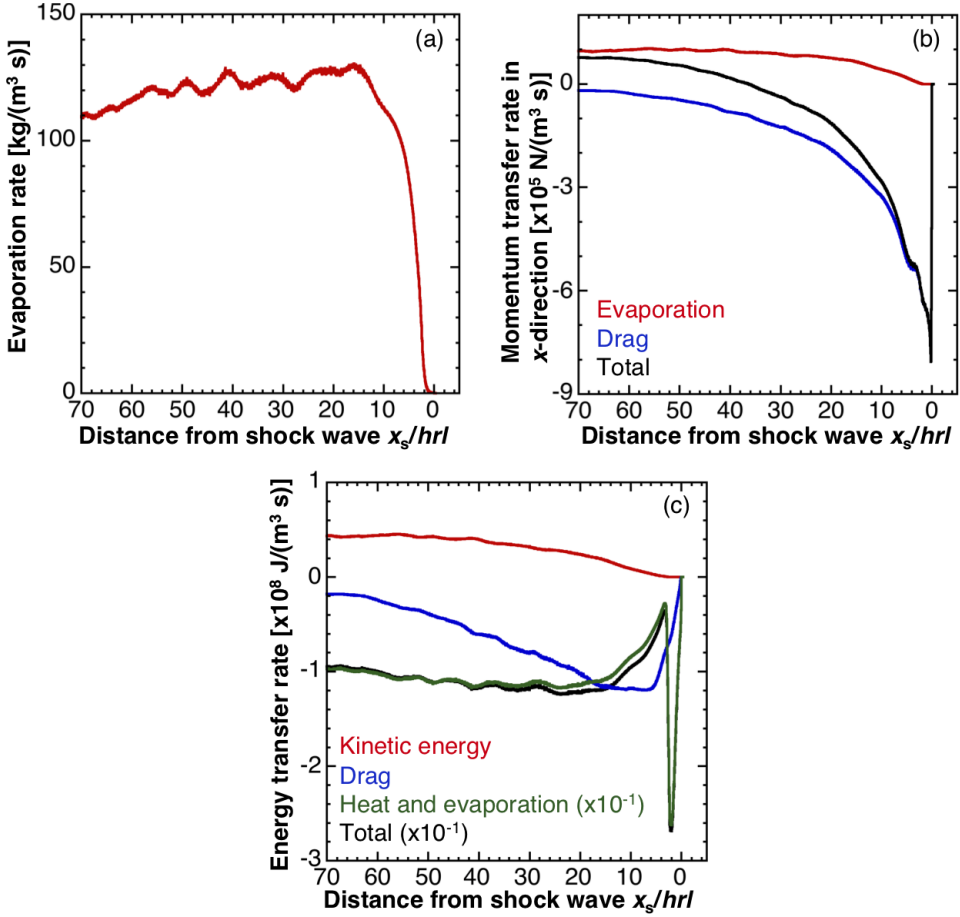


FIGURE 14. Favre averaged interphase exchange rates from mean values. (a) Evaporation rate, (b) Momentum transfer rate, (c) Energy transfer rate

The profile of momentum transfer rate in Fig. 14(b) is similar to that of the drag force in Fig. 10(e), the maximum being located at the detonation front. However, two factors for the momentum transfer are present: the first is due to drag and the second is due to evaporation. The former decreases as the relative velocity decreases and the latter contributes to increase the gas momentum.

The energy transfer is composed of three contributions (Fig. 14(c)). The first is due to the kinetic energy of the evaporating droplets, the second is due to the work of drag and the third which is the main contribution is due to the convective heat transfer and evaporation. The transferred kinetic energy increases due to the increase of the velocity of droplet (Fig. 11(b)). The drag work is maximum at some distance from the shock. Indeed, the droplet has to get some velocity so that the drag work is non-zero. The peak of the energy transfer is due to the heat transferred to the droplets to attain the saturation temperature. The amount of the energy transfer associated with endothermic evaporation is proportional to the amount of the evaporated WDs (Figs. 14(a)(c)).

The interphase exchanges will modify the gaseous flux. From the mean values, the mass, momentum and total enthalpy gaseous flux have been evaluated and shown in Fig. 15, in line with Radulescu *et al.* (2007). As for the gaseous mass flux, the density and velocity have opposite trends but the overall flux increases by several percent (Fig. 15(a)). The



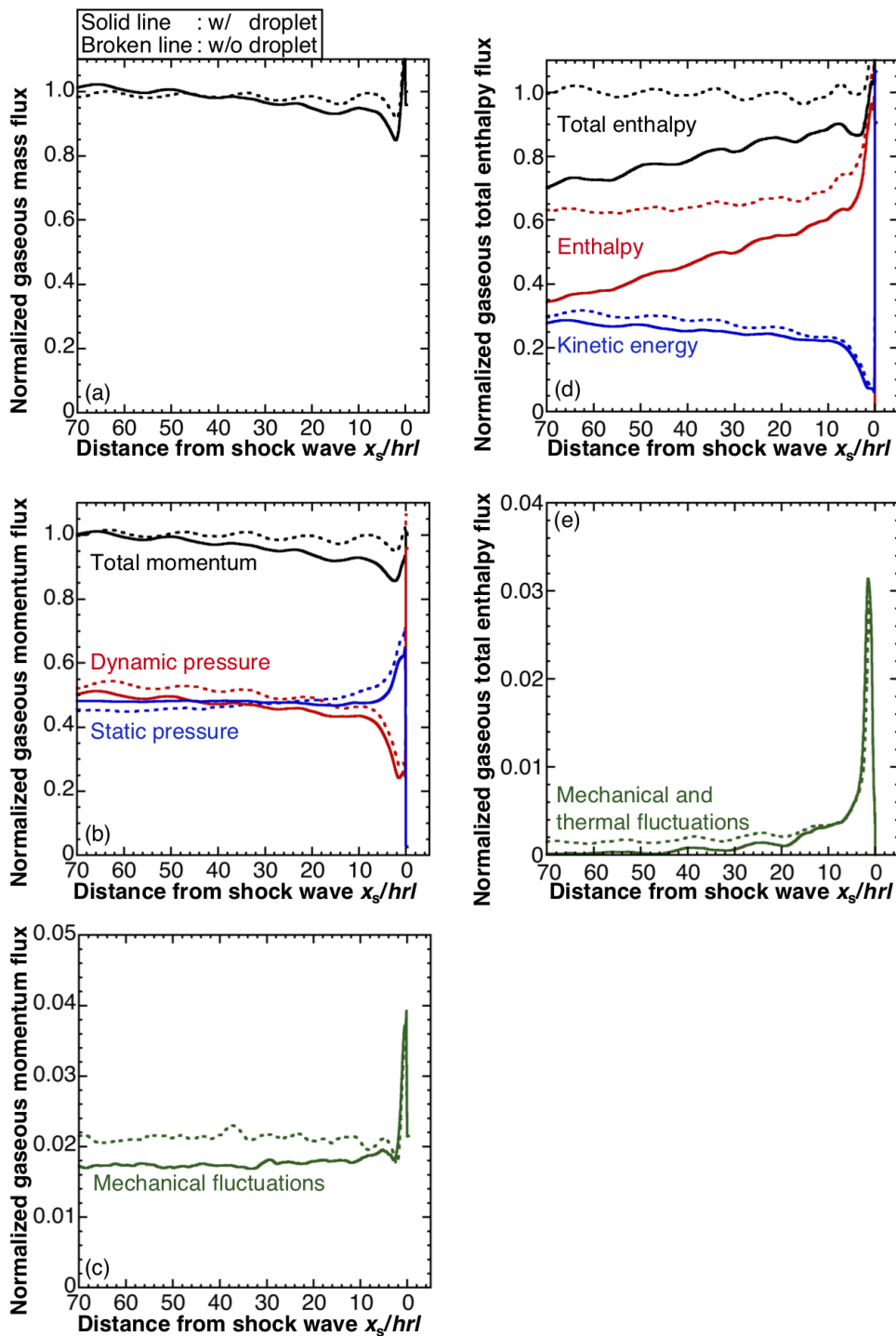


FIGURE 15. Computed gaseous flux from averaged values. (a) Gaseous mass flux, (b) Gaseous momentum flux, (c) Mechanical fluctuations in the gaseous momentum flux, (d) Gaseous total enthalpy flux, (e) Mechanical and thermal fluctuations in the gaseous total enthalpy flux

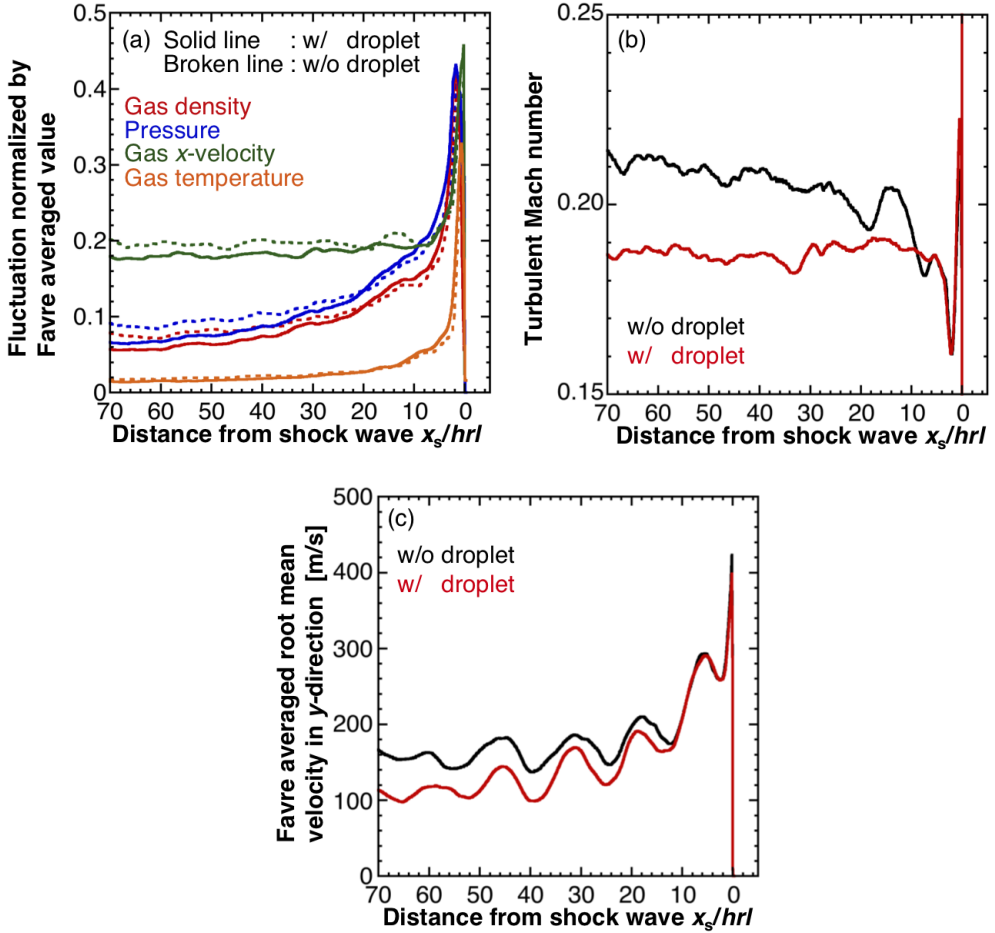


FIGURE 16. Favre averaged profile on fluctuation. (a) Fluctuation normalized by Favre averaged value, (b) Turbulent Mach number, (c) Favre averaged root mean gas velocity in  $y$ -direction

overall gaseous momentum flux of the wet case is less than the dry case (Fig. 15(b)), mainly due to drag, which surpasses the evaporation contribution (Fig. 14(b)). The dynamic pressure of the wet case is lower than the dry case. The wet static pressure is lower at the shock due to the detonation velocity decrease, and then gets higher after some distance due to the relaxation processes. As for the gaseous total enthalpy flux, all contributions decrease (Fig. 15(d)). Near the shock, the contribution of enthalpy to the total enthalpy is very high, then a first decrease to 75% can be observed. Indeed, below 5  $hrl$ , the gas has to bring the droplets to their saturation temperature. Then, the total enthalpy continues to decrease more smoothly, due to drag and evaporation. The relative contribution of the enthalpy which decreases to 60% in the dry case, decreases up to 40% in the wet case, which means that the energy transfer mainly acts on the enthalpy. Thus in our case, the ratio of the enthalpy to the kinetic energy greatly decreases near the sonic line, as compared to the pure gaseous case.

Regardless of the presence of the WDs, the mechanical fluctuations in total momentum flux take a peak value of about 4% compared to the gaseous momentum flux just after the shock wave and then remains relatively constant in the rear (Fig. 15(c)). The mechanical

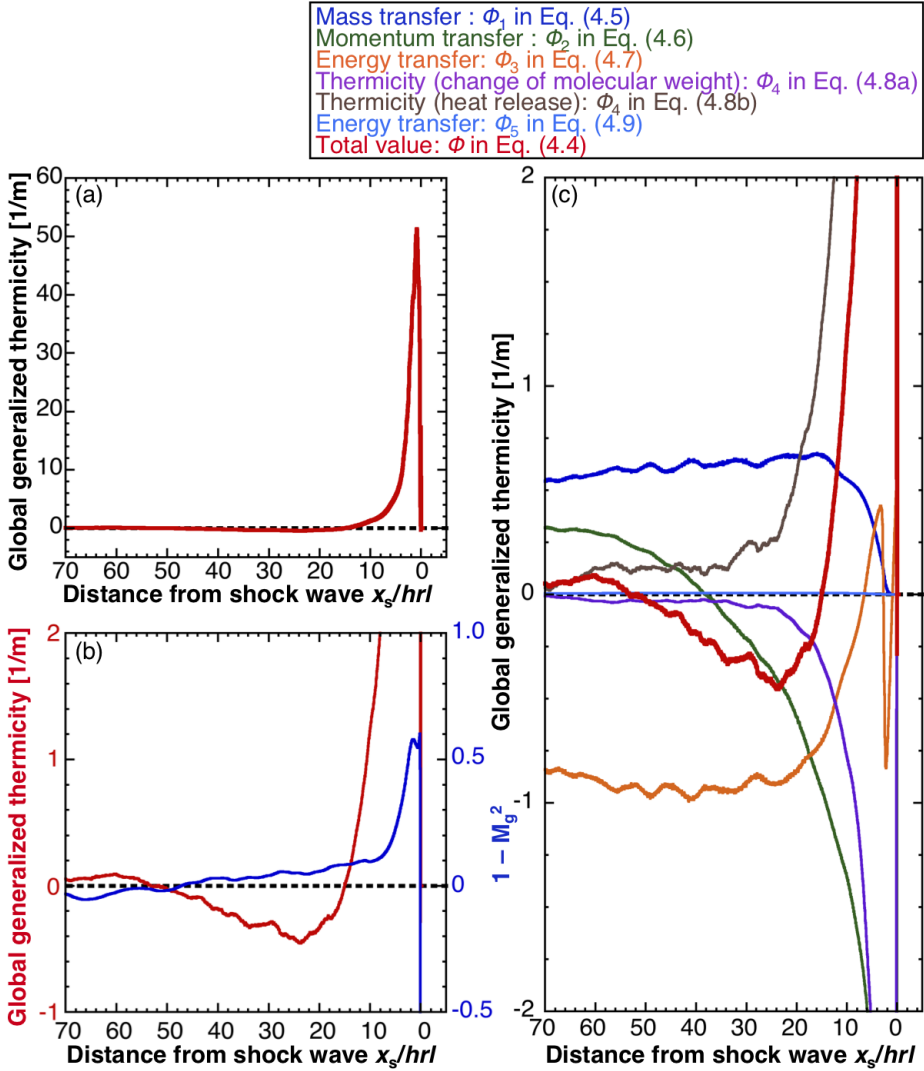


FIGURE 17. Global generalized thermicity for gaseous detonations laden with inert WDs. (a) Global generalized thermicity, (b) Close-up view of global generalized thermicity and gas Mach number, (c) Contribution of each term of the global generalized thermicity of the Master equation (ME<sup>2</sup>) Eq. (4.4)

fluctuations for gaseous detonation with WDs are lower than that without WDs behind the shock wave. The mechanical and thermal fluctuations in total enthalpy flux are suppressed with the presence of WDs as shown in Fig. 15(e). Indeed, drag of droplets, of which size is smaller than the eddy size will naturally decrease the level of velocity fluctuations.

To obtain more insight into the lowering of fluctuations, Fig. 16 shows (a) Favre averaged fluctuations in gas quantities normalized by Favre averaged value and (b) Favre averaged turbulent Mach number, (c) Favre averaged root mean gas velocity in  $y$ -direction. Here, the turbulent Mach number is defined as the ratio of the fluctuations in gas velocity in the  $x$ -direction to the gas sound speed. After a first peak, the momentum transfer between phases decreases the gas  $y$ -velocity (Fig. 16(c)). Also, fluctuations of gas

density, pressure, gas velocity in  $x$ -direction and gas temperature take their maximum value just behind the front, and reach equilibrium (Fig. 16(a)), of which value is lower with WDs. In addition, the turbulent Mach number gradually approaches 0.19 and 0.21 in the rear for the case with and without WDs, respectively (Fig. 16(b)). This implies that the existence of WDs lowers the turbulence. From the above, the interphase transfer moderates the gradient of the physical quantity and the WDs play a role in lowering the overall fluctuations.

As the liquid volume fraction and the level of fluctuations are very low, the following laminar Master Equation for gaseous detonations laden with inert WDs (ME<sup>2</sup>) can be derived from Higgins (2012), Zhang (2009) and Lee (2008).

$$(1 - M_g^2) \frac{1}{u_g} \frac{du_g}{dx} = \Phi \quad (4.4)$$

$$\Phi = \Phi_1 + \Phi_2 + \Phi_3 + \Phi_4 + \Phi_5$$

The "global generalized thermicity" can be decomposed into the following five contributions.

$$\Phi_1 = \frac{\dot{m}}{\rho_g u_g} \quad (4.5)$$

$$\Phi_2 = \frac{1}{p_g} [\dot{F} - (D - u_g)\dot{m}] \quad (4.6)$$

$$\Phi_3 = \frac{1}{\rho_g u_g c_{p,g} T_g} \left[ \dot{E} + \frac{D^2}{2} \dot{m} - D\dot{F} - \dot{m} \left( h_g + \frac{u_g^2}{2} \right) \right] \quad (4.7)$$

$$\Phi_4 = \Phi_{4a} + \Phi_{4b} \quad (4.8)$$

$$\Phi_{4a} = -\frac{1}{u_g W_g} \frac{dW_g}{dt} \quad (4.8a)$$

$$\Phi_{4b} = -\frac{1}{u_g c_{p,g} T_g} \sum_k \frac{\dot{\omega}_{g,k}}{\rho_g} h_k \quad (4.8b)$$

$$\Phi_5 = -\frac{1}{\rho_g u_g c_{p,g} T_g} \sum_k h_{g,k} (\dot{m}_k - Y_{g,k} \dot{m}) \quad (4.9)$$

Here  $\rho_g$ ,  $u_g$ ,  $T_g$ ,  $M_g$ ,  $h_g$ ,  $c_{p,g}$  and  $W_g$  are gas density, gas  $x$ -velocity in the shock frame, gas temperature, Mach number based on gas sound speed, gas enthalpy, specific heat at constant pressure for gas phase and gas molar mass, respectively. In this equation,  $\dot{m}$ ,  $\dot{F}$  and  $\dot{E}$  represent the right-hand side of Eqs. (2.1)-(2.3) and  $D$  is the mean detonation velocity obtained from the simulations. The first term (Eq. 4.5) is related to the evaporation mass transfer. The second term (Eq. 4.6) is related to the momentum transfer. The third term (Eq. 4.7) and fifth term (Eq. 4.9) translate the influence of the energy transfer. The fourth term (Eq. 4.8) is the classical thermicity term due to molar change (Eq. ??a) and chemical heat release (Eq. ??b). On Fig. 17, the global generalized thermicity  $\Phi$  (Eq. 4.4), which is here the right-hand side of ME<sup>2</sup> shows a non-monotonous behavior. It becomes zero at 15 *hrl*, at approximately the same location where the Mach number based on the two-phase sound speed goes to one. The global thermicity is also zero at 53 *hrl*, where the Mach number based on the gas sound speed  $M_g$  goes to one (Figs. 17(a)(b)).

However, the two-phase sound speed is not completely relevant in our case, as there is still a pronounced velocity disequilibrium. Thus, the Master Equation ME<sup>2</sup> shows that

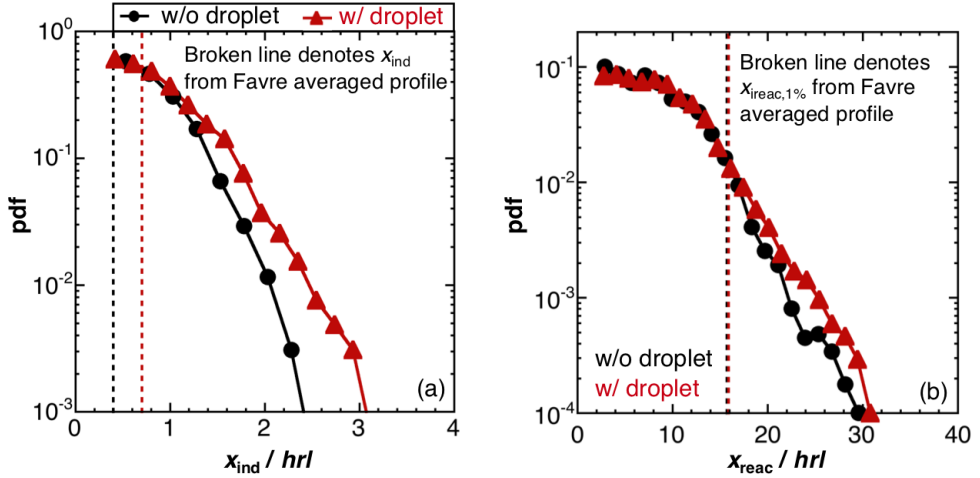


FIGURE 18. Variation in induction and reaction zone length. (a) Probability density function for induction length defined by maximum thermicity position, (b) Probability density function for reaction length defined by the position where the thermicity is 1% of the maximum value.

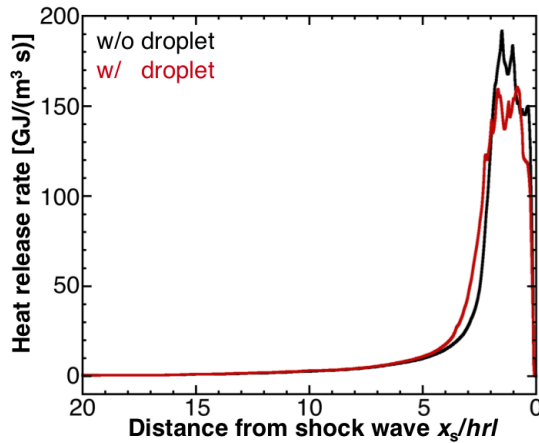


FIGURE 19. Computed heat release rate from mean values as a function of distance

the hydrodynamic thickness should rely on the gaseous sound speed, due to the fact that the group velocity of the pressure waves is probably close to that of the gas pressure wave velocity. Moreover, this laminar Master equation, works well, as the working mixture is a weakly unstable one and that the cell becomes more regular with WDs addition. From the contribution of each term in the Master Equation  $ME^2$  around the mean sonic point by gas sound speed (Fig. 17(c)), energy transfer by WDs decreases the gas velocity whereas the mass, momentum and chemical reactions play a role in accelerating the gas.

#### 4.6. Effect of water vapor from evaporation on chemistry

The additional water vapor from evaporation of WDs may modify the chemical path of the gaseous detonation. The pdf of the induction and reaction lengths during propagation are depicted in Fig. 18. Owing to a lower detonation velocity, the probability to get greater induction lengths increases (Figs. 8(j) and 18(a)). However, the pdf of the reaction length is almost the same regardless of the presence of WDs (Figs. 8(j) and 18(b)). Figure 19

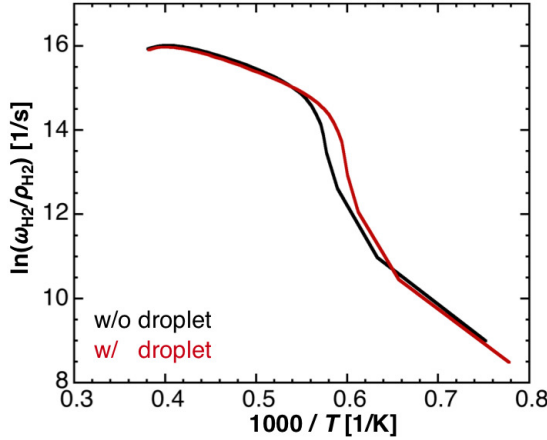


FIGURE 20. Computed reaction rate of  $H_2$  from mean values as a function of mean temperature

depicts the heat release rate computed from the mean values  $\sum_k \dot{\omega}_{g,k} h_{g,k}$ . The peak is decreased and the width is thickened, with WDs addition.

In order to quantify the influence of additional water vapor on the reactivity of the mixture, Fig. 20 shows the Arrhenius plot for hydrogen computed from the mean values. The chemical reaction starts from lower temperature than that without WDs due to the decrease of the propagation velocity. However, the slope is the same regardless of the presence of the WDs, which means that the global activation energy in the induction and reaction zones does not change by WDs.

Indeed, from comparison of the characteristic length for induction zone and breakup in the previous sub-sections, the breakup occurs downstream of the induction zone. Thus, the water vapor from the evaporation of WDs does not affect the reactivity of the gaseous detonation in our case, as the amount of water coming from WDs evaporation within the induction zone is small (see Figs. 8(h)(j) and 10(c)).

#### 4.7. Comparison of the characteristic lengths

In this section, the mean structure of gaseous detonation with WDs is explained by comparing the characteristic lengths of gaseous detonation and that of WDs obtained in previous sections.

The characteristic lengths for gaseous detonation are the induction length, reaction length and the hydrodynamic thickness. The induction length is more or less increased (0.4 - 3.4  $hrl$ ) due to lower propagation velocity, whereas the reaction length remains almost the same between the dry and wet case, about 15  $hrl$  (see Section 4.6). Based on the gas sound speed, the hydrodynamic thickness increased from 33 to 47  $hrl$  (Section 4.3).

The two-phase interactions between the gas and WDs inside the mean subsonic zone between the mean shock location and the sonic surface induce the decrease of detonation propagation velocity. The temperature of the droplet rapidly reaches the saturation temperature at 3  $hrl$ . Then, breakup which occurs and ends at 5  $hrl$  will produce smaller droplets, enhancing the overall interphase exchanges. However, the breakup is performed mostly after the induction zone. Thus, the additional water vapor which is produced during evaporation does not influence the main reaction zone. Only a drop of gas temperature is inferred from this endothermic evaporation. The latter proceeds well

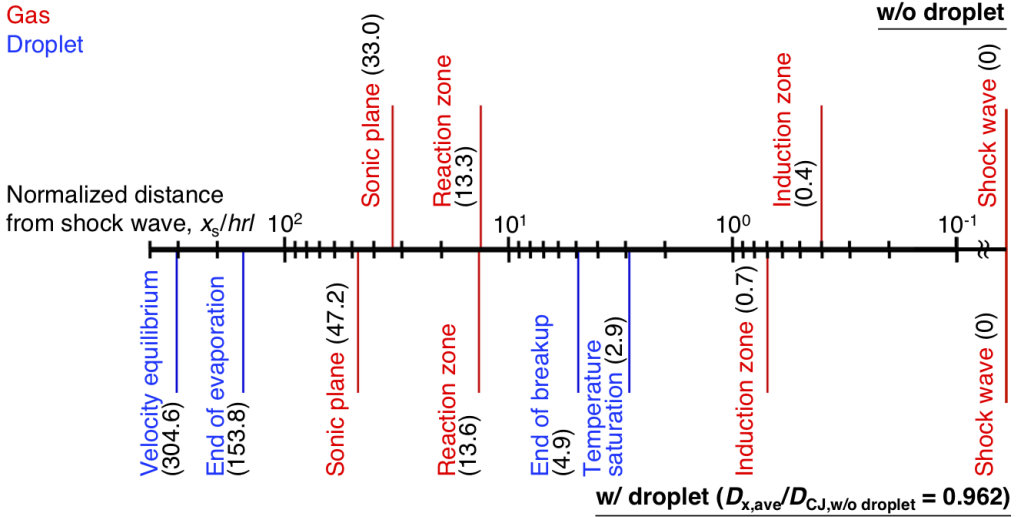


FIGURE 21. Schematic of gaseous detonation with dilute water spray under present simulation conditions

after the sonic plane and at the end, velocity equilibrium is also achieved. On the other hand, thermal equilibrium is not achieved.

Under the present simulation conditions, the schematic of gaseous detonation with dilute WDs based on the present analysis is shown in Fig. 21 and the characteristic lengths of detonation and interphase exchanges can be ordered as follows:  $x_{ind} < x_{sat} < x_{br} < x_{reac} < x_{HT} < x_{evap} < x_{eq,velo}$ . These characteristic lengths are intimately intertwined and characterize the mean structure of steady gaseous detonation laden with WDs.

The present finding is thus in line with one of the limits exhibited by Jarsalé's experiments (Jarsalé 2017) when the induction zone is shorter than the secondary breakup length and that the additional water vapor produced does not influence the main reaction zone, even if the mixtures are different.

## 5. Conclusions

The mean structure of gaseous detonation with dilute water spray was numerically analyzed using two-dimensional reactive Navier-Stokes equations with detailed chemistry and Eulerian-Lagrangian method. The present simulation takes into account droplet breakup which plays a crucial role in interphase exchanges and behavior of WDs. The gaseous detonation with dilute water spray is studied using the recycling block method to enable detonation to propagate long distance with an aim to get the statistical values. Its structure is qualitatively revealed by 2D flow fields and more quantitatively by the Favre averaged profiles in time and space for the dry and wet cases. The cellular structure of gaseous detonation with dilute water spray is more regular than the dry gaseous detonation counterpart, even if the cell size does not change much. Also, the flow fields reveal less complicated structures and the level of the fluctuations that develop downstream of the leading shock is lowered. However, the hydrodynamic thickness, based on the gas sound speed is increased due to the interaction with water spray, probably due to the cooling process of evaporation and the energy transfer. The global two-phase exchanges (mass, momentum and energy) that occur within the subsonic zone, induce a decrease of the detonation velocity. Droplet breakup occurs downstream of the induction

zone and in our case, the water vapor from evaporation of the spray does not affect the reactivity of the gaseous detonation. Moreover, the mean particle Reynolds and Weber numbers have enabled us to characterize the regimes of droplet motion and the breakup regimes, which depend on the initial pressure. From the particle Mach number, immediately after the shock, the droplet experiences supersonic flows and then relaxes to subsonic conditions. In addition, the ratio of the enthalpy to that of the total enthalpy is decreased as compared to the dry case, increasing the relative importance of the kinetic energy. The laminar Master Equation which has been derived shows that the hydrodynamic thickness should rely on the gaseous sound speed, and works well as the working mixture is a weakly unstable one and its cellular structure is regular.

The characteristic lengths of detonation and interphase exchanges have been ordered under the present simulation conditions and have been shown to be intimately intertwined.

## Acknowledgements

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## Appendix A. Detailed chemical reaction mechanism by Hong, Davidson & Hanson (2011)

The chemical reaction used in the present paper is the detailed chemical reaction mechanism proposed by Hong, Davidson & Hanson (2011), which considers 9 species and 20 elementary reactions. The chemical reaction mechanism is listed in Table 3.

## Appendix B. Validation case: interaction of a shock wave with a cloud of water droplets

The validation for the present numerical model on the droplet breakup is conducted through the comparison with previous experiment and simulation on the interaction of a shock wave with a cloud of water droplets.

### B.1. Computational target

The reference experiment has been conducted by Chauvin *et al.* (2011). Figure 22 shows the schematic of the experiments, as well as the initial conditions for the computations. They used a vertical shock tube with a total length of 3795 mm and an inner square cross section of 80 mm aside. The high-pressure chamber is 750 mm long and the driven section is 3045 mm. The test section at atmospheric conditions is filled with a cloud of droplets which is located between 2970 mm and 3710 mm. In the simulations, the droplet



No.	Reaction	$A$	$n$	$E_a$
1	$\text{H} + \text{O}_2 = \text{OH} + \text{O}$	1.04E+14	0.0	15286
2	$\text{H} + \text{O}_2 (+\text{H}_2\text{O}) = \text{H}_2\text{O} (+\text{H}_2\text{O})^b$	5.59E+13	0.2	0
	Low-pressure limit	3.70E+19	-1.0	0
	$\text{H} + \text{O}_2 (+\text{O}_2) = \text{H}_2\text{O} (+\text{O}_2)^a$	5.59E+13	0.2	0
	Low-pressure limit	5.69E+18	-1.1	0
	$\text{H} + \text{O}_2 (+\text{M}) = \text{H}_2\text{O} (+\text{M})^a$	5.59E+13	0.2	0
	Low-pressure limit	2.65E+19	-1.3	0
	Collider efficiency ( $\text{N}_2 = 1$ ): $\text{H}_2 = 1.5, \text{H}_2\text{O} = 0, \text{O}_2 = 0$			
3	$\text{H}_2\text{O}_2 (+\text{M}) = 2\text{OH} (+\text{M})^c$	8.59E+14	0	48560
	Low-pressure limit	9.55E+15	0	42203
	Collider efficiency : $\text{N}_2 = 1.5, \text{H}_2\text{O} = 9$			
4	$\text{OH} + \text{H}_2\text{O}_2 = \text{H}_2\text{O} + \text{HO}_2$	1.74E+12	0.0	318
	$\text{OH} + \text{H}_2\text{O}_2 = \text{H}_2\text{O} + \text{HO}_2$	7.59E+13	0.0	7269
5	$\text{OH} + \text{HO}_2 = \text{H}_2\text{O} + \text{O}_2$	2.89E+13	0	-500
6	$\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$	1.30E+11	0	-1603
	$\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$	4.20E+14	0	11980
7	$\text{H}_2\text{O} + \text{M} = \text{H} + \text{OH} + \text{M}$	6.06E+27	-3.31	120770
	Collider efficiency : $\text{H}_2\text{O} = 0, \text{H}_2 = 3, \text{N}_2 = 2, \text{O}_2 = 1.5$			
	$\text{H}_2\text{O} + \text{H}_2\text{O} = \text{H} + \text{OH} + \text{H}_2\text{O}$	1.00E+26	-2.44	120160
8	$\text{OH} + \text{OH} = \text{H}_2\text{O} + \text{O}$	3.57E+04	2.4	-2111
9	$\text{O} + \text{H}_2 = \text{H} + \text{OH}$	3.82E+12	0	7948
	$\text{O} + \text{H}_2 = \text{H} + \text{OH}$	8.79E+14	0	19170
10	$\text{H}_2 + \text{OH} = \text{H}_2\text{O} + \text{H}$	2.17E+08	1.52	3457
11	$\text{H} + \text{HO}_2 = \text{OH} + \text{OH}$	7.08E+13	0	300
12	$\text{H} + \text{HO}_2 = \text{H}_2\text{O} + \text{O}$	1.45E+12	0	0
13	$\text{H} + \text{HO}_2 = \text{H}_2 + \text{O}_2$	3.66E+06	2.087	-1450
14	$\text{O} + \text{HO}_2 = \text{OH} + \text{O}_2$	1.63E+13	0	-445
15	$\text{H}_2\text{O}_2 + \text{H} = \text{HO}_2 + \text{H}_2$	1.21E+07	2.0	5200
16	$\text{H}_2\text{O}_2 + \text{H} = \text{H}_2\text{O} + \text{OH}$	1.02E+13	0	3577
17	$\text{H}_2\text{O}_2 + \text{O} = \text{OH} + \text{HO}_2$	8.43E+11	0	3970
18	$\text{H}_2 + \text{M} = \text{H} + \text{H} + \text{M}$	5.48E+18	-1.1	104380
	Collider efficiency : $\text{H}_2\text{O} = 14.4$			
	$\text{H}_2 + \text{H}_2 = \text{H} + \text{H} + \text{H}_2$	9.03E+14	0	96070
	$\text{H}_2 + \text{N}_2 = \text{H} + \text{H} + \text{N}_2$	4.58E+19	-1.4	104380
	$\text{H}_2 + \text{O}_2 = \text{H} + \text{H} + \text{O}_2$	4.58E+19	-1.4	104380
19	$\text{O} + \text{O} + \text{M} = \text{O}_2 + \text{M}$	6.16E+15	-0.5	0
	Collider efficiency ( $\text{N}_2 = 1$ ): $\text{H}_2 = 2.5, \text{H}_2\text{O} = 12$			
20	$\text{O} + \text{H} + \text{M} = \text{OH} + \text{M}$	4.71E+18	-1.0	0
	Collider efficiency ( $\text{N}_2 = 1$ ): $\text{H}_2 = 2.5, \text{H}_2\text{O} = 12$			

<sup>a</sup>  $F_{\text{cent}} = 0.7$

<sup>b</sup>  $F_{\text{cent}} = 0.8$

<sup>c</sup>  $F_{\text{cent}} = 1.0$

TABLE 3.  $\text{H}_2/\text{O}_2$  reaction mechanism by Hong, Davidson & Hanson (2011).  
 $k = AT^n \exp(E_a/RT)$  in unit of  $[\text{s}^{-1}]$ ,  $[\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}]$  or  $[\text{cm}^6 \text{mol}^{-2} \text{s}^{-1}]$

distribution is uniform, with a mean diameter of 500  $\mu\text{m}$ . The liquid volume fraction is 1%. Two pressure transducers are placed at 3080 mm and 3520 mm, which lie within the cloud. The Mach number is 1.49, thus the pressure in the driver section is 0.68 MPa. The mesh is uniform with a grid size of 1 mm and one-dimensional unsteady simulation is performed. The simulation without breakup is also conducted and is compared with the case that takes breakup into account to highlight its influence.

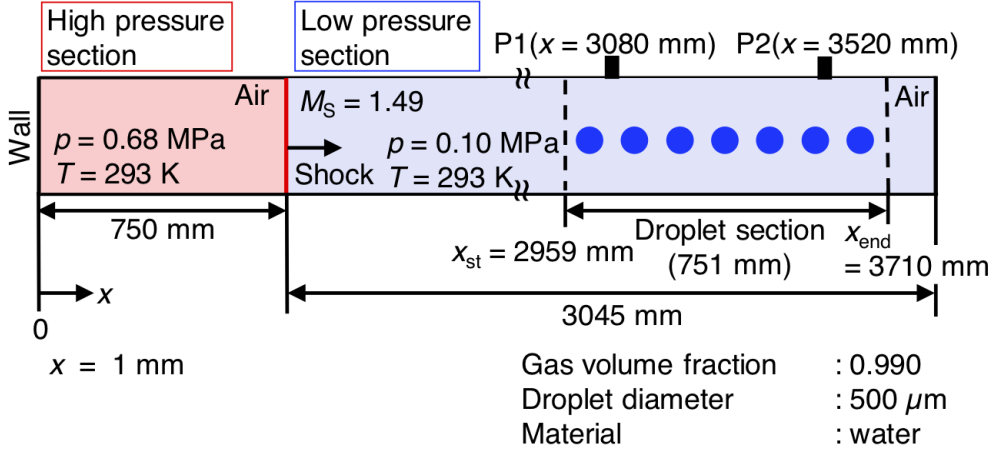


FIGURE 22. Interactions of a shock wave with a cloud of droplets. Initial conditions of the interaction of shock wave with a cloud of droplets

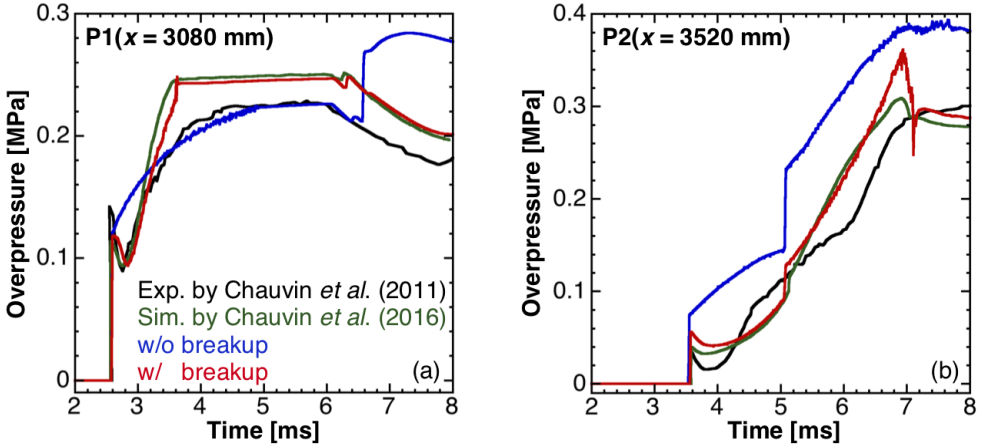


FIGURE 23. Comparison of the overpressure evolution at two locations in the cloud of droplets between the experimental and numerical results. (a) first transducer P1 at  $x = 3080$  mm, (b) second one P2 at  $x = 3520$  mm

## B.2. Overpressure history

The evolution of the overpressure in present simulation is compared to experimental and numerical results of Chauvin *et al.* (2011) and Chauvin *et al.* (2016) in order to validate the implementation of the model. Figure 23 shows the overpressure history (a) of P1 the first pressure transducer at  $x = 3080$  mm, (b) and P2 the second one at  $x = 3520$  mm, inside the water cloud. The initial time in Fig. 23 is the time when the shock wave reaches  $x = 1770$  mm in the experiment. The simulation with breakup in Fig. 23 can capture the main features observed in the experiment that is, the overpressure decreases just after the shock wave passage and then relaxes to its equilibrium value. Indeed, droplet breakup greatly increases the interphase exchanges between phases, thus decreasing the gaseous velocity. The induced expansion decreases the overpressure, which also decreases the shock velocity driven by the gaseous phase. The simulation shows the same trend in overpressure after the passage of the shock wave as in the experiment. Also, the comparison between the present simulation with breakup based on Eulerian-

Eulerian method and the previous simulation results with the Marble model (Chauvin *et al.* 2016) shows good agreement. Therefore, the present simulation reproduces the phenomena of the interaction of the shock wave with a water cloud, thus validating the breakup model. On the other hand, the simulation without breakup overestimates the overpressure history and shows a completely different trend. These comparisons show that the breakup modeling plays an important role in post-shock two-phase flows.

### Appendix C. Assessment of numerical convergence

The numerical uncertainty is assessed by comparing the simulation results in the coarser grid in this section. The grid width used in the main result is 50  $\mu\text{m}$  and that for the coarse grid is twice more, that is 100  $\mu\text{m}$ . The simulation conditions are the same as presented in Section 3. The gaseous detonation with dilute water spray propagates steadily and the decrease in mean propagation velocity compared to CJ velocity without WDs is 3.8%.

In order to assess the robustness of the main conclusions on mean structure by characteristic length comparison in Fig. 21, the Favre averaged one-dimensional profiles for gas phase in the coarse grid are shown in Fig. 24, which shows (a) pressure, (b) gas density, (c) Mach number in the mean shock frame, (d) thermicity, respectively. From Fig. 24, the profiles for gas phase globally show the same tendency between the present and coarse grid. The characteristic lengths for the gas phase are estimated in the same manner as in Section 4.3 and listed in Table 4. Moreover, although the value of the characteristic length for gas phase becomes slightly lower in the coarse grid, the ordering among the different characteristic lengths for gas phase is not affected by the grid resolution.

Figure 25 shows the Favre averaged one-dimensional profiles for water droplets, (a) droplet diameter, (b) Weber number, (c) droplet mass ratio, (d) velocity in  $x$ -direction, respectively. The profiles for Weber number between the two grid show similar trend and the time for WDs to finish breakup is longer in the coarse grid (Fig. 25(b)). The numerical resolution influences the degree of droplet breakup and then the diameter at the breakup process is larger in the coarse grid (Fig. 25(a)). After the breakup completion, the droplet diameter gradually decreases only by the evaporation and the droplet mass ratio is higher in the coarse grid, which comes from the slower evaporation process by larger droplet diameter (Figs. 25(a)(c)). From the view point of the velocity equilibrium, water droplets with larger diameter in the coarse grid take slightly longer time to accelerate due to smaller surface area (Fig. 25(d)). However, the general feature for the velocity profiles is captured in the coarse grid. The characteristic lengths for water droplets are estimated in the same manner as in Section 4.4 and listed in Table 5. The characteristic lengths for water droplet are elongated in the coarse grid due to the change in behavior of droplet diameter in Fig. 25(a). Nevertheless, the grid resolution does not change the sequence of the characteristic lengths for water droplets.

The mean quantities for gas phase are converged and mean behavior of water droplets are similar between the fine present grid and the coarse grid. Therefore, the main conclusions on the mean structure for gaseous detonation with dilute WDs will not be changed by the numerical uncertainty.

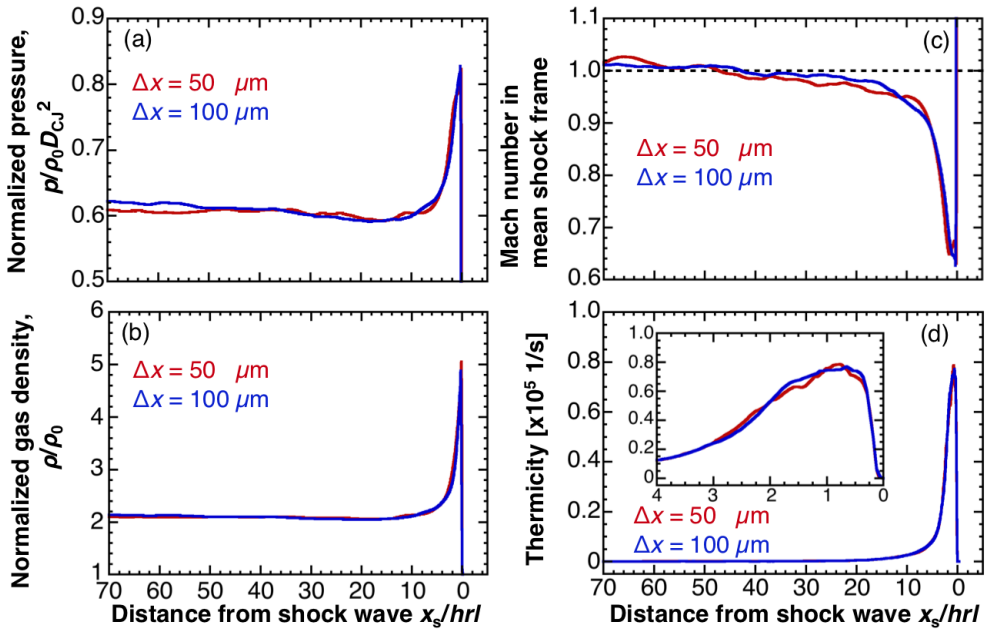
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	w/ droplet (50 $\mu\text{m}$ )	w/ droplet (100 $\mu\text{m}$ )
$x_{\text{ind,themicity}}$	0.7	0.6
$x_{\text{ind,OH}}$	3.4	2.8
$x_{\text{reac,1\%}}$	15.9	15.9
$x_{\text{reac,max}}$	13.6	13.6 (gas sound speed based)
$x_{\text{HT,gas}}$	47.2	42.8

 TABLE 4. Characteristic lengths for gaseous detonation (normalized by  $h_{rl}$ ) in coarse grid

	w/ droplet (50 $\mu\text{m}$ )	w/ droplet (100 $\mu\text{m}$ )
$x_{\text{sat}}$	2.9	3.1
$x_{\text{br}}$	4.9	5.5
$x_{\text{eq,velo}}$	304.6	376.0
$x_{\text{evap}}$	153.8	194.1

 TABLE 5. Characteristic lengths for liquid dispersed phase (normalized by  $h_{rl}$ ) in coarse grid

 FIGURE 24. Favre averaged profiles for gas phase in the coarse grid (100  $\mu\text{m}$ ). (a) Pressure, (b) Gas density, (c) Mach number in mean shock frame, (d) Thermicity

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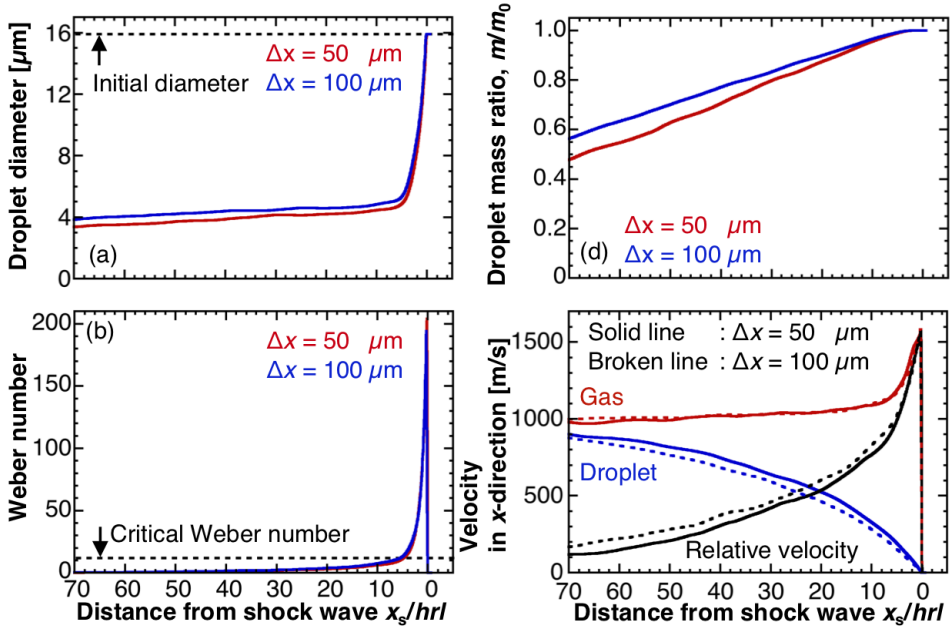


FIGURE 25. Favre averaged profiles for water droplet in the coarse grid (100  $\mu\text{m}$ ). (a) Droplet diameter, (b) Weber number, (c) Droplet mass ratio, (d) Velocity in  $x$ -direction

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