Interactions between Propagating Ammonia/Hydrogen-Air Detonation and Ammonia Spray Cloud

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1. Introduction

Hydrogen combustion is a clean, powerful, and efficient energy conversion process, but there are concerns about its safety, including issues of leakage, autoignition, and explosion. Compared to hydrogen, ammonia, as a zero-carbon fuel, shows superiority in storage and transport, but its characteristics of low reactivity, high ignition energy, and slow burning velocity limit its applications. Ammonia/hydrogen blends can overcome some above-mentioned drawbacks in pure hydrogen and pure ammonia fuels and are expected to be part of future clean energy propulsion systems. Detonative combustion in gaseous ammonia/hydrogen blends displays higher pressure and temperature compared to deflagration, and thus lower NOx emissions are expected [1]. Low pollutant emissions (i.e., NO) observed in detonated mixtures indicate the potential of using ammonia/hydrogen blends in detonation-based engines [2].

Direct injection and subsequent combustion of ammonia sprays has been proposed to mitigate equipment and operating costs and the start-up time of ammonia fuelled engines. Okafor et al. [3,4] took the lead in reporting successful combustion of liquid ammonia spray co-fired with a gaseous promoter fuel (i.e., methane) in a novel gas turbine swirl combustor. Due to the high latent heat of ammonia vaporisation with flash boiling effects, ammonia vaporisation was not immediately complete after injection, though preheated air and recirculation of heat and active radicals were utilised to compensate for the large cooling effects. A spray cloud of ammonia droplets was observed at the flame base, which might inhibit the stability of ammonia spray flames. To further provide scientific understanding, more detailed information on interactions between combustion and an ammonia spray cloud is required but difficult to be measured.

This study aims to understand the physics of how liquid-phase ammonia spray cloud affects gas-phase ammonia/hydrogen blends' detonative combustion by a numerical methodology. The effects of ammonia droplet size and concentration on detonation diffraction and re-initiation are discussed.

4. Ongoing Work

- Ammonia clouds with small droplet size and large concentration trigger detonation diffraction and re-initiation, and extremely high pressure are recorded.
- ☐ To further analyse the shock focusing mechanism of detonation diffraction and re-initiation
- The stability of detonative combustion is disturbed, but detonation extinction is not found.
- ☐ To investigate if ammonia spray cloud can cause detonation extinction
- For cases with large ammonia droplet size or low ammonia droplet concentration, detonation propagation is almost undisturbed or slightly disturbed.
- ☐ To discuss effects of ammonia cloud size on detonation propagation

2. Methodology

OpenFOAM CFD solver: RYrhoCentralFoam-dev

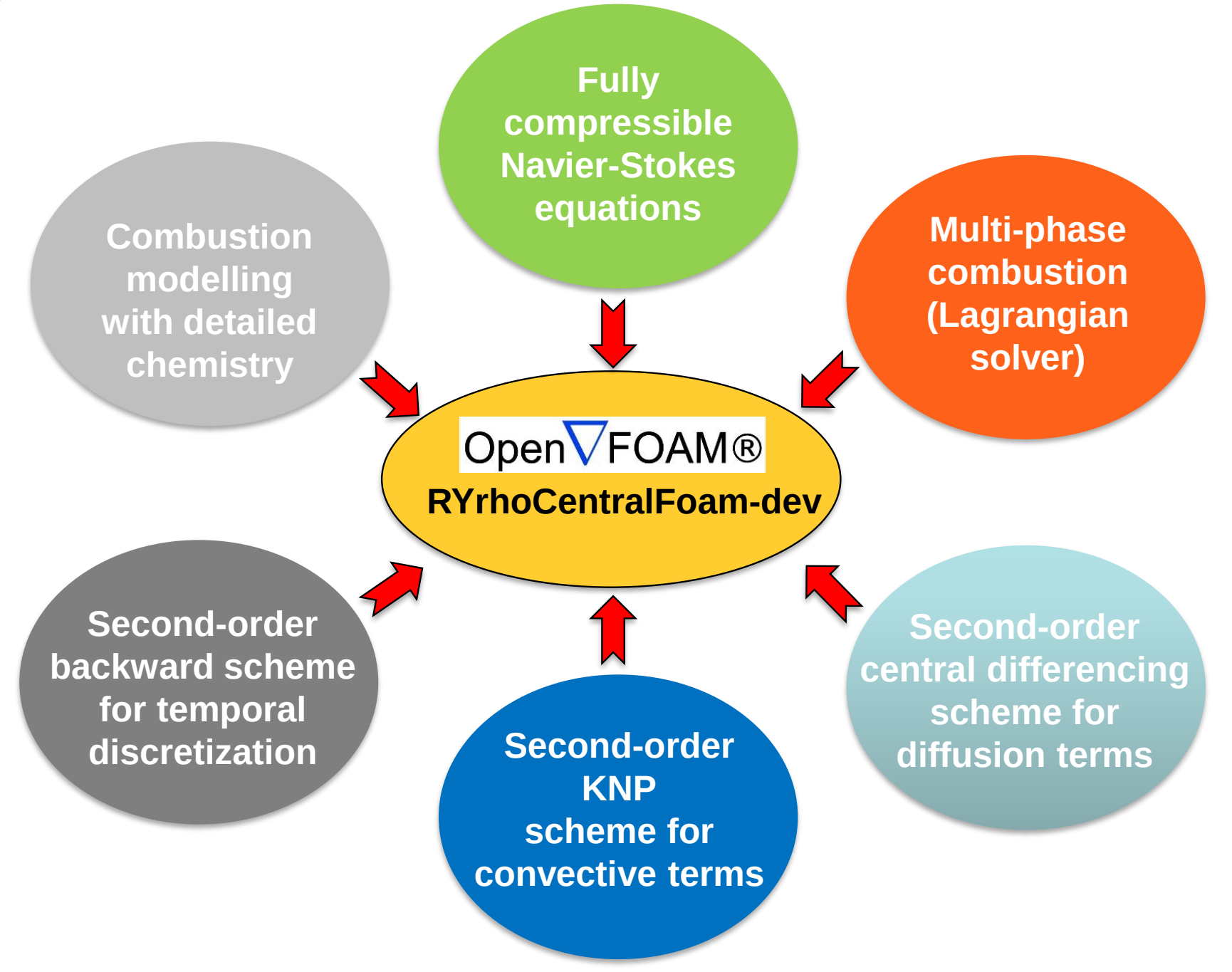

FIG. 1. The RYrhoCentralFoam-dev solver and numerical algorithms.

OpenFOAM dev
The OpenFOAM Foundation

- New version of RYrhoCentralFoam [5] developed based on OpenFOAM dev to implement thermophysical properties of liquid ammonia
- Hybrid Eulerian-Lagrangian flow solver based on semi-discrete and central-upwind Kurganov, Noelle, and Petrova (KNP) scheme
- Extensively validated in shock capturing, shock-eddy-flame interactions, single droplet evaporation, gas-liquid coupling, etc

Eulerian solver for gas phase

Compressible governing equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = S_{\mathrm{mass}}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \big(\mathbf{u}(\rho \mathbf{u})\big) + \nabla p - \nabla \cdot \hat{\tau} = \mathbf{S}_{\mathrm{momentum}}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot \big(\mathbf{u}(\rho E + p)\big) - \nabla \cdot (\mathbf{u} \cdot \hat{\tau}) - \nabla \cdot (k \nabla T) = \dot{\omega}_T + S_{\mathrm{energy}}$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot \big(\mathbf{u}(\rho Y_i)\big) - \nabla \cdot (\rho D \nabla Y_i) = \dot{\omega}_i + S_{\mathrm{species},i}, \quad (i = 1, \cdots, N)$$

- $\hat{\tau}$: viscous stress tensor; $\dot{\omega}_T$: combustion heat release; $\dot{\omega}_i$: net production rate of i -th species

Lagrangian solver for liquid phase

Two-phase exchange terms:

$$S_{\mathrm{mass}} = -\frac{1}{V_c} \sum_{1}^{N_d} \dot{m}_d$$

$$\mathbf{S}_{\mathrm{momentum}} = -\frac{1}{V_c} \sum_{1}^{N_d} (\mathbf{F}_d + \mathbf{F}_p)$$

$$S_{\mathrm{energy}} = -\frac{1}{V_c} \sum_{1}^{N_d} (\dot{Q}_c + \dot{Q}_{\mathrm{lat}})$$

$$S_{\mathrm{species},i} = \begin{cases} S_{\mathrm{mass}}, \text{for condensed species} \\ 0, \text{for other species} \end{cases}$$

Equations of a single droplet:

$$\frac{dm_d}{dt} = -\dot{m}_d$$

$$\frac{d\mathbf{u}_d}{dt} = \frac{\mathbf{F}_d + \mathbf{F}_p}{m_d}$$

$$c_{p,d} \frac{dT_d}{dt} = \frac{\dot{Q}_c + \dot{Q}_{\mathrm{lat}}}{m_d}$$

- $\mathbf{F}_d$: drag force; $\mathbf{F}_p$: pressure gradient force; $\dot{Q}_c$: convective heat transfer; $\dot{Q}_{\mathrm{lat}}$: latent heat transfer

- Lagrangian solver computes dispersed ammonia droplets with hybrid Lagrangian particle tracking and stochastic parcel methods
- Droplets are grouped into parcels and share identical properties, e.g., diameter, density, temperature, etc
- Individual parcels are treated as Lagrangian points and tracked for mass, velocity, energy and location

5. References

1. H. Xiao, A. Valera-Medina and P. J. Bowen. Modeling combustion of ammonia/hydrogen fuel blends under gas turbine conditions. Energy & Fuels, 31(8):8631–8642, 2017.
2. R. Zhu, X. Fang, C. Xu, M. Zhao, H. Zhang and M. Davy. Pulsating one-dimensional detonation in ammonia-hydrogen–air mixtures. International Journal of Hydrogen Energy, 47(50):21517–21536, 2022.
3. E. C. Okafor, H. Yamashita, A. Hayakawa, K. D. K. A. Somarathne, T. Kudo, T. Tsujimura, M. Uchida, S. Ito, and H. Kobayashi. Flame stability and emissions characteristics of liquid ammonia spray co-fired with methane in a single stage swirl combustor. Fuel, 287:119433, 2021.
4. E. C. Okafor, O. Kurata, H. Yamashita, T. Inoue, T. Tsujimura, N. Iki, A. Hayakawa, S. Ito, M. Uchida, and Hideaki Kobayashi. Liquid ammonia spray combustion in two-stage micro gas turbine combustors at 0.25 MPa; Relevance of combustion enhancement to flame stability and NOx control. Applications in Energy and Combustion Science, 7:100038, 2021.
5. Z. Huang, M. Zhao, Y. Xu, G. Li and H. Zhang. Eulerian-Lagrangian modelling of detonative combustion in two-phase gas-droplet mixtures with OpenFoam: Validations and verifications. Fuel, 286:119402, 2021.
6. Y. Xu and H. Zhang. Interactions between a propagating detonation wave and circular water cloud in hydrogen/air mixture. Combustion and Flame, 245:112369, 2022.

3. Results

Physical model and parametric studies

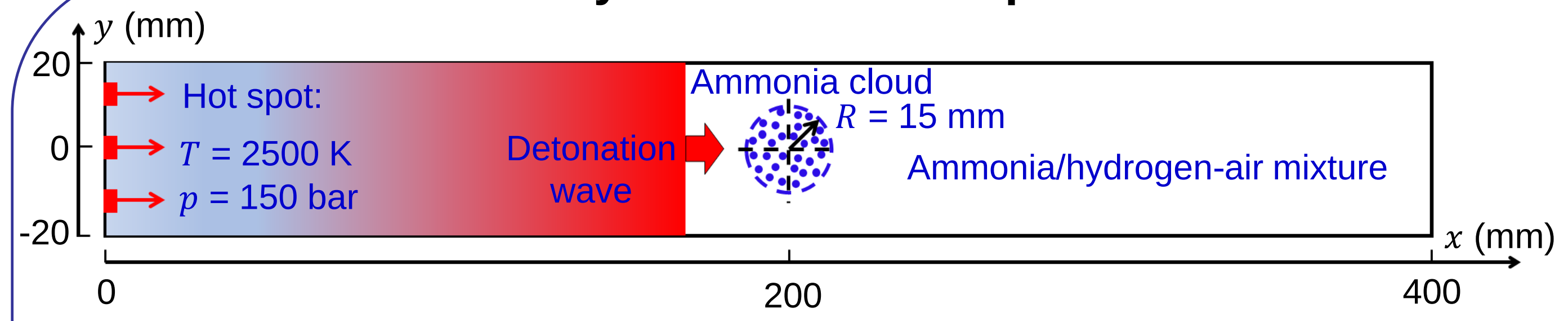

FIG. 2. Schematic of the computational domain [6]. Blue dots: ammonia droplets.

- Fuel: NH_3-H_2 molar ratio 3:7
- T_0 = 300 K, P_0 = 2 bar
- Spray cloud: mono-sized NH_3 droplets

TABLE1. Tracking of parametric numerical experiments. C1: base case.

Case	Droplet diameter (d_0) (μm)	Droplet concentration (C_0) (kg/m³)	Phenomenon
C0	N.A.	0	N.A.
C1	2.5	0.51	Detonation diffraction and re-initiation
C2	5	0.51	Detonation diffraction and re-initiation
C3	10	0.51	Almost undisturbed detonation propagation
C4	2.5	2.04	Detonation diffraction and re-initiation
C5	2.5	0.13	Disturbed detonation propagation

Detonation diffraction and re-initiation

- DW: detonation wave
- RF: reaction front
- SF: shock front
- AS: auto-ignition spot

- **Autoignition spot:** almost along the centreline due to focusing of the upper and lower parts of SF
- Ammonia droplets break up and evaporate into gaseous ammonia as the inner SF compresses and heats the cloud
- No residual liquid ammonia, but small pockets of unburned gaseous ammonia upstream of the RF

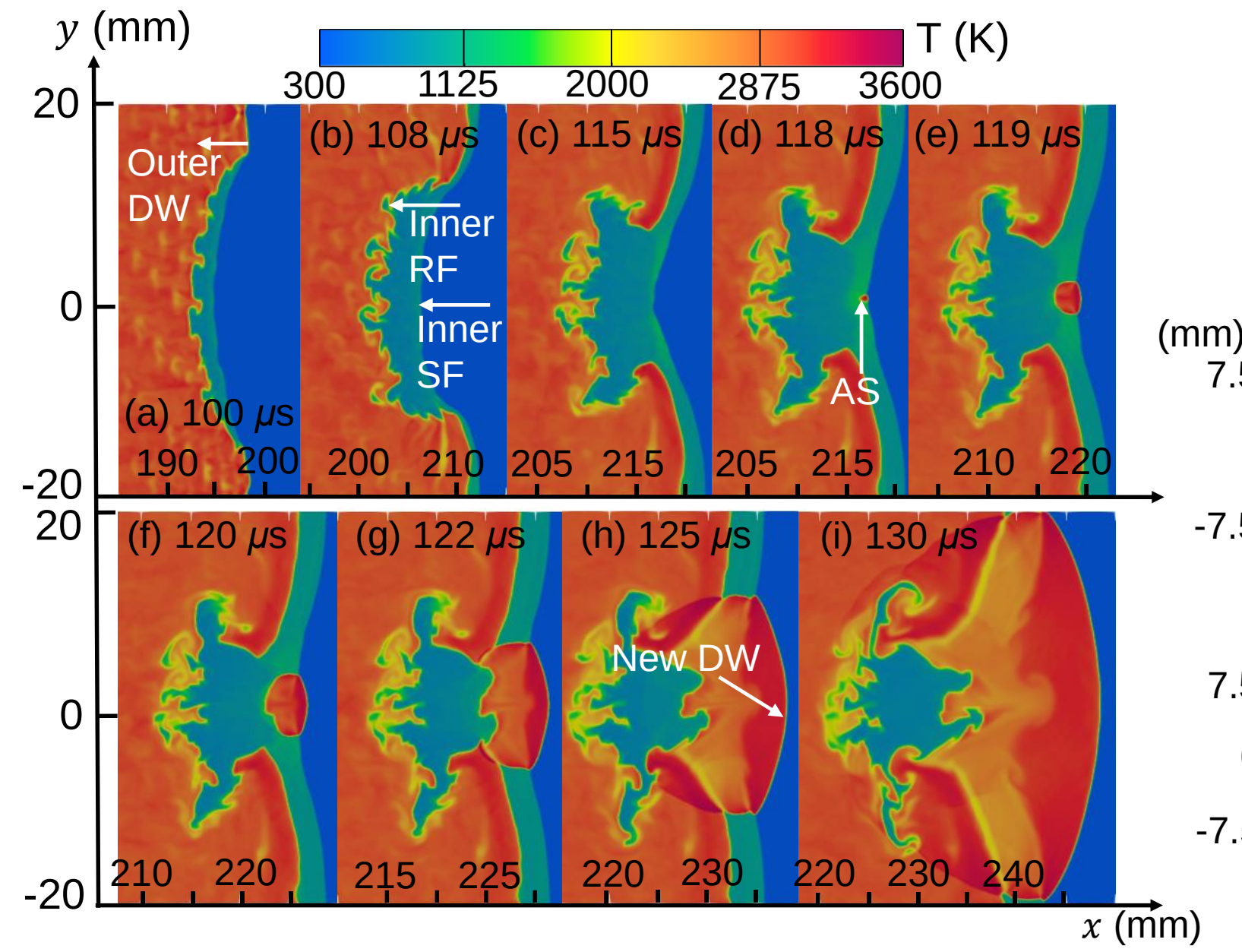

FIG. 4. Evolutions of gas temperature in detonation diffraction and re-initiation. Results from Case C1: $C_0 = 0.51\ \mathrm{kg/m^3}$, $d_0 = 2.5\ \mu\mathrm{m}$.

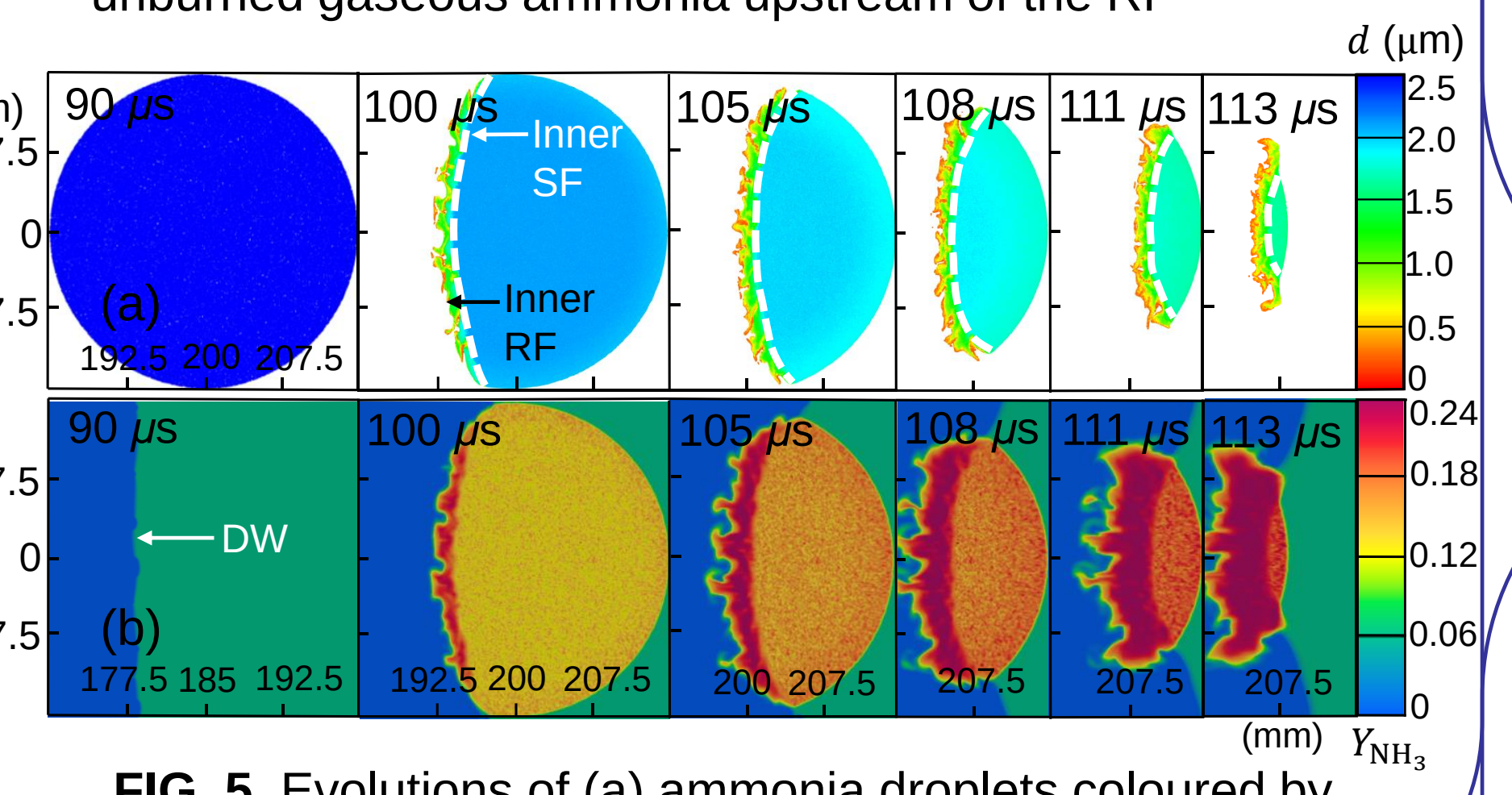

FIG. 5. Evolutions of (a) ammonia droplets coloured by diameter and (b) gaseous ammonia mass fraction. Dashed curves: inner shock front. Results from Case C1.

Effects of ammonia droplet concentration

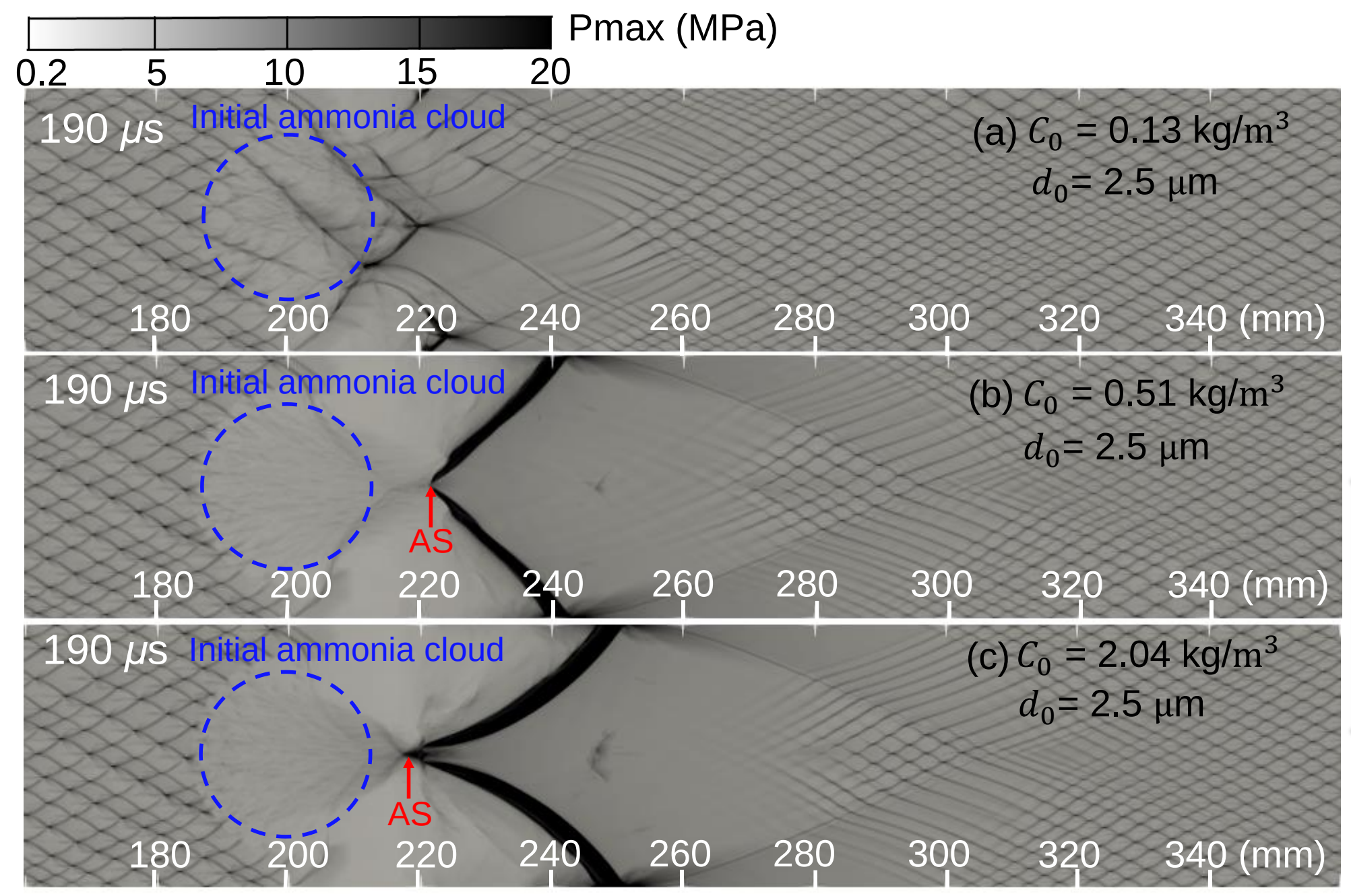

FIG. 7. Trajectories of peak pressure with various droplet diameters. Results from Cases C1, C4, C5: $d_0 = 2.5\ \mu\mathrm{m}$.

- Disturbed detonation propagation
- No detonation diffraction observed, and the regularity of cellular detonative front soon restored
- Detonation diffraction and re-initiation

Gaseous detonation propagation

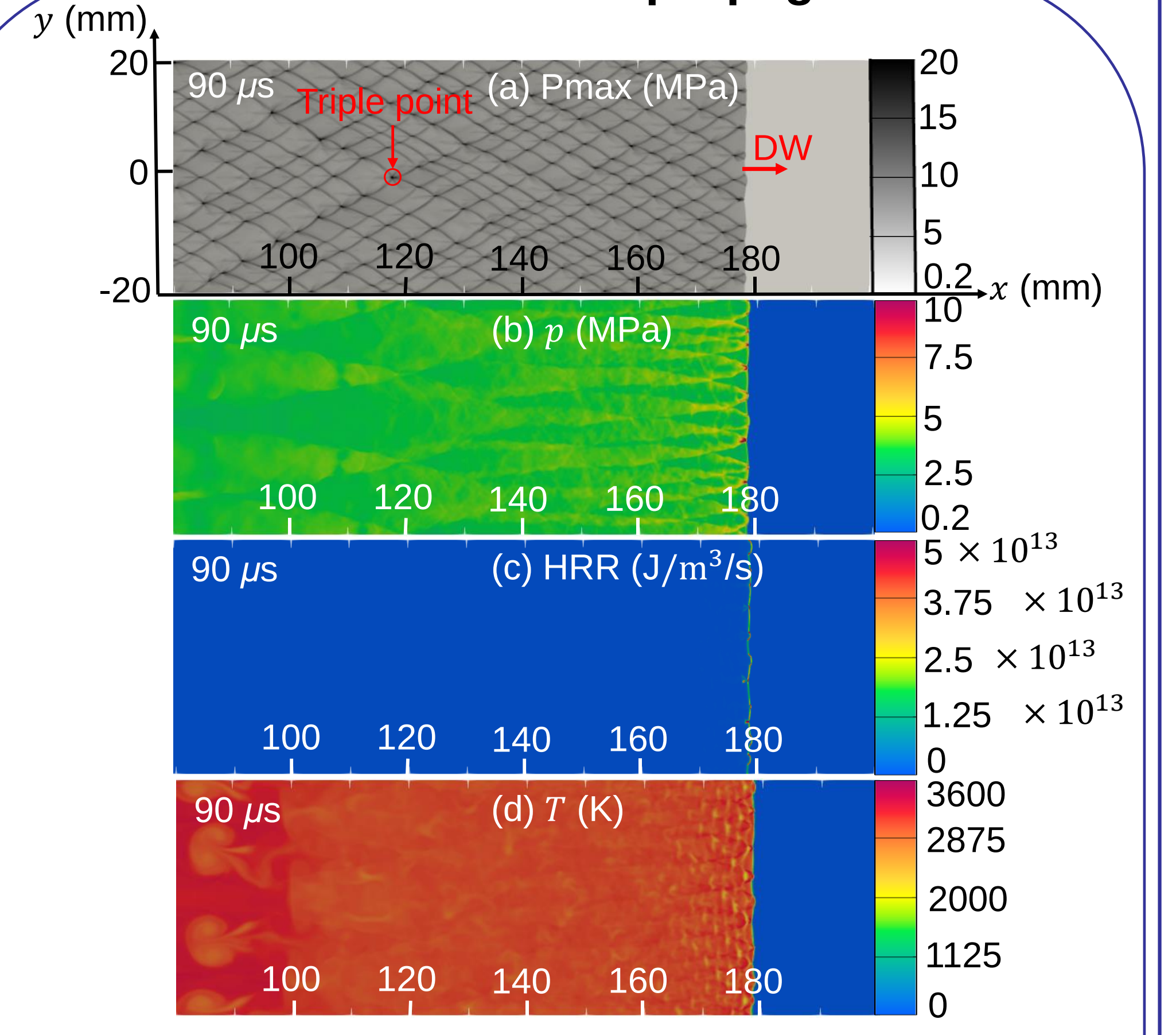

FIG. 3. Distributions of (a) peak pressure trajectory, (b) pressure, (c) heat release rate and (d) temperature for detonation propagation in the gaseous mixture. Results from Case C0. DW: detonation wave.

- Pmax: the history of maximum pressure during detonation propagation, corresponds to the trajectory of triple points
- Cellular detonative front: triple points connecting transverse wave, incident wave, Mach wave and shear layer

Effects of ammonia droplet size

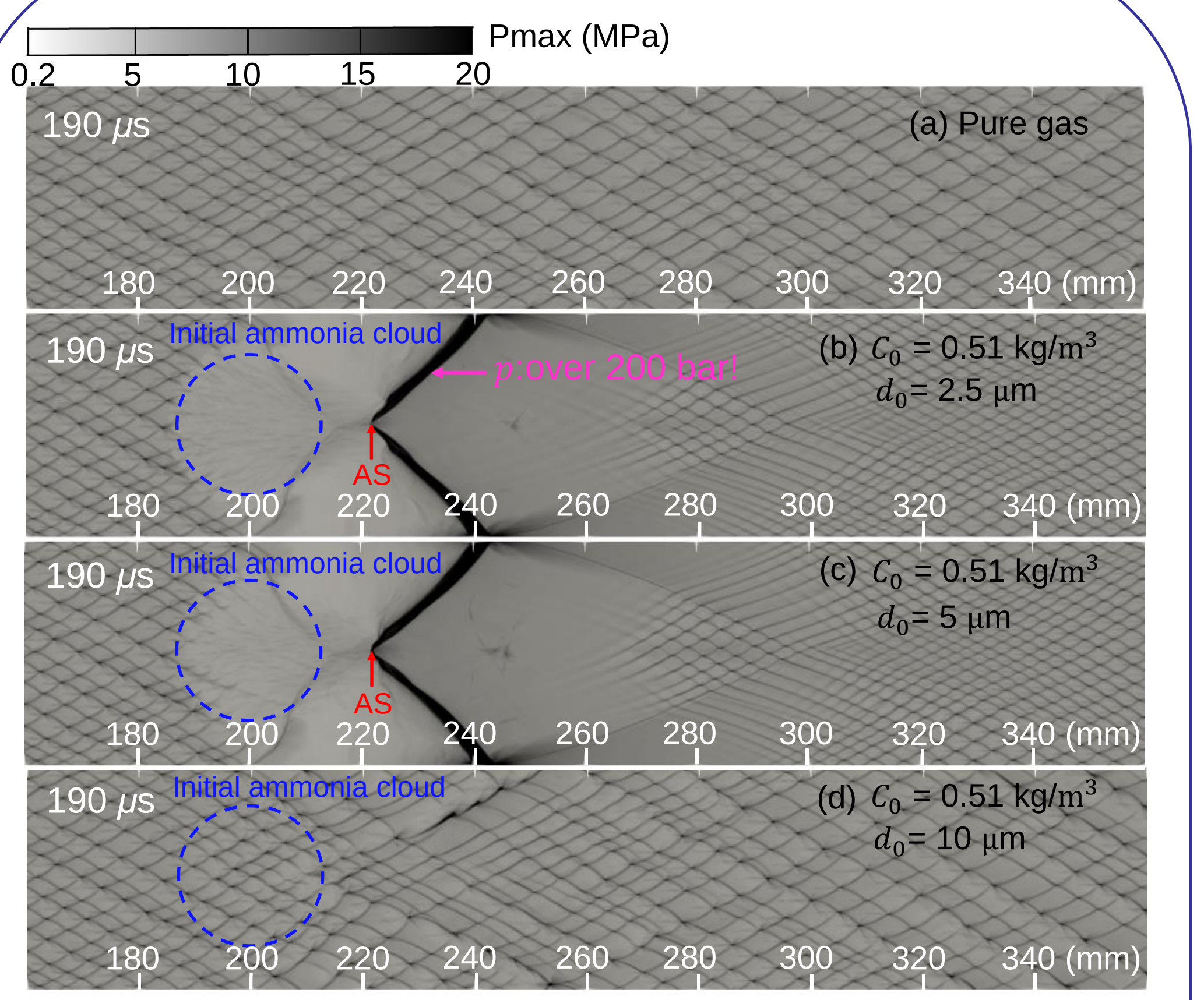

FIG. 6. Trajectories of peak pressure with various droplet diameters. Results from Cases C1, C2, C3: $C_0 = 0.51\ \mathrm{kg/m^3}$.

- (b)-(c): detonation diffraction and re-initiation; increased averaged cell width in the post-cloud area after detonation re-initiation, i.e., enhanced frontal instability of new DW
  - (d): almost undisturbed detonation propagation