Flame acceleration, detonation limit and heat loss for hydrogen-oxygen mixture at cryogenic temperature of 77 K

Xiaobo Shen, Wenju Fu, Jiayu Shen and Jennifer X Wen

j.wen@surrey.ac.uk

ICHS International Conference on Hydrogen Safety
Québec
ICHS2023

UNIVERSITY OF SURREY

FEMG Fire and Explosion Modelling Group

Institute for Sustainability
UNIVERSITY OF SURREY

華東理工大學
EAST CHINA UNIVERSITY OF SCIENCE AND TECHNOLOGY

Contents

- Background
- Previous works
- Experimental setup
- Results
- Concluding remarks

Fire and Explosion Modelling Group

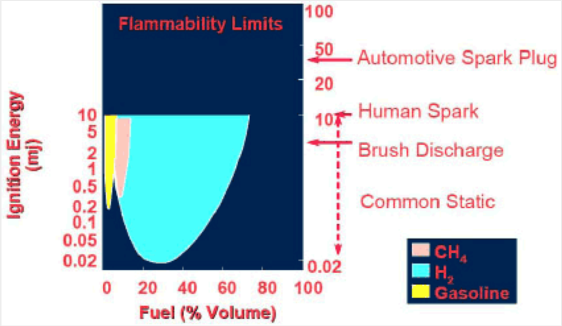
Background

https://www.rivieramm.com/news-content-hub/news-content-hub/review-hydrogen-as-a-marine-fuel-74697

https://www.energy.gov/eere/fuelcells/liquid-hydrogen-delivery

https://newatlas.com/aircraft/h2fly-liquid-hydrogen-flight/

- Confined spaces
- Pipelines
- Tunnels…



https://qtxasset.com/files/sensorsmag/nodes/2008/1481/Figure1.gif

Limited knowledge about how flame accelerates and detonates at cryogenic temperatures

Fire and Explosion Modelling Group

Previous study

- **Gaseous hydrogen (ambient conditions)**
  - Manson and Guénoche, 1957. Kuznetsov et al., 2005 (Boundary layer effect)
  - Kogarko and Zeldovich, 1948 (Minimum criterion for detonation $d_{min} = \lambda/\pi$)
  - Dorofeev et al., 2001, 2007 (Critical condition between strong and weak flame acceleration)

- **Gaseous hydrogen (cryogenic conditions)**
  - Kuznetsov et al., 2021 (90-130 K, H2-air, various equivalence ratios)
  - Shen et al., 2022 (77K, H2-O2, equivalence ratio 2.6)

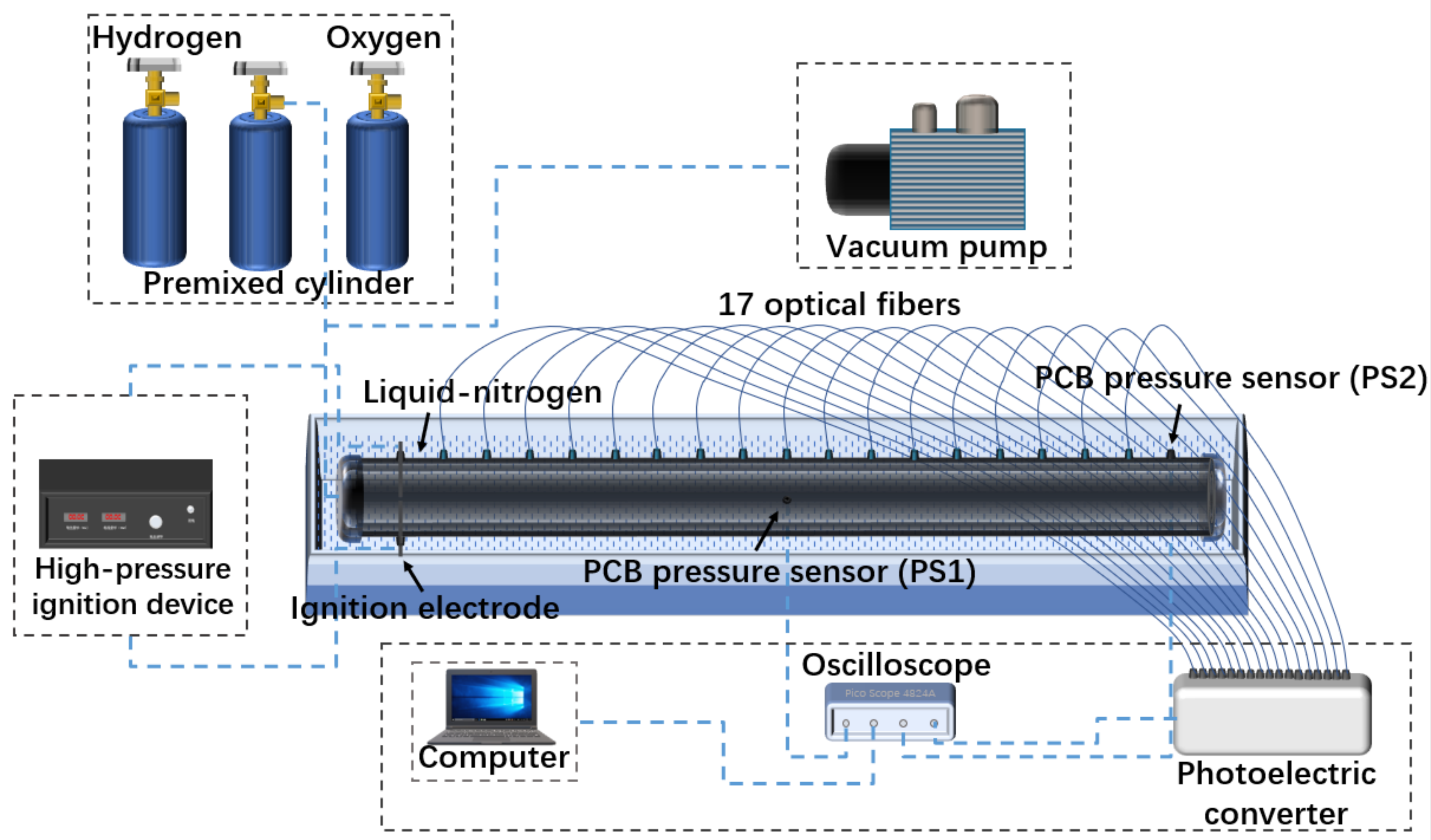
The mechanism of flame acceleration and detonation cell regularity at cryogenic conditions?

Kuznetsov, M., Denkevits, A., Veser, A., Friedrich, A., Necker, G. and Jordan, T., Shock tube experiments on flame propagation regimes and critical conditions for flame acceleration and detonation transition for hydrogen-air mixtures at cryogenic temperatures, Int. Conf. on Hydrogen Safety, 2021.

Shen, X., Fu, W., Liang, W., Wen, J.X., Liu, H. and Law, C.K., Strong flame acceleration and detonation limit of hydrogen-oxygen mixture at cryogenic temperature, Proceedings of the Combustion Institute, 2022.

Fire and Explosion Modelling Group

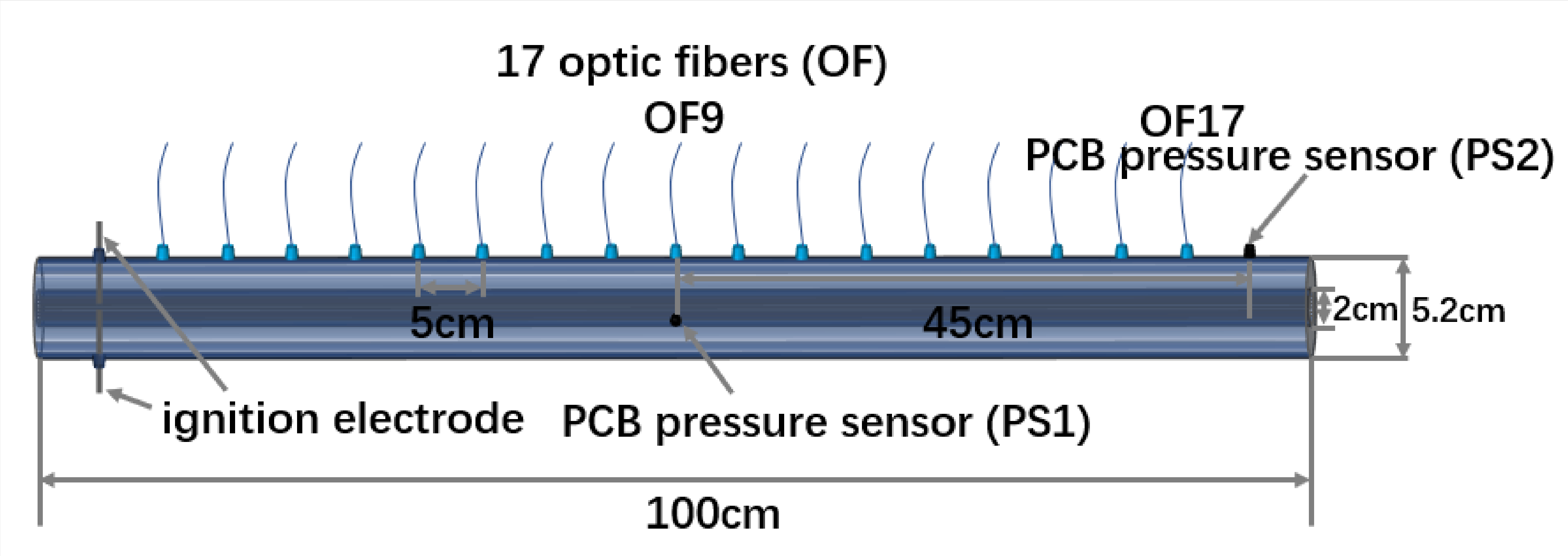
Experimental Setup



Schematic diagram of experimental device.

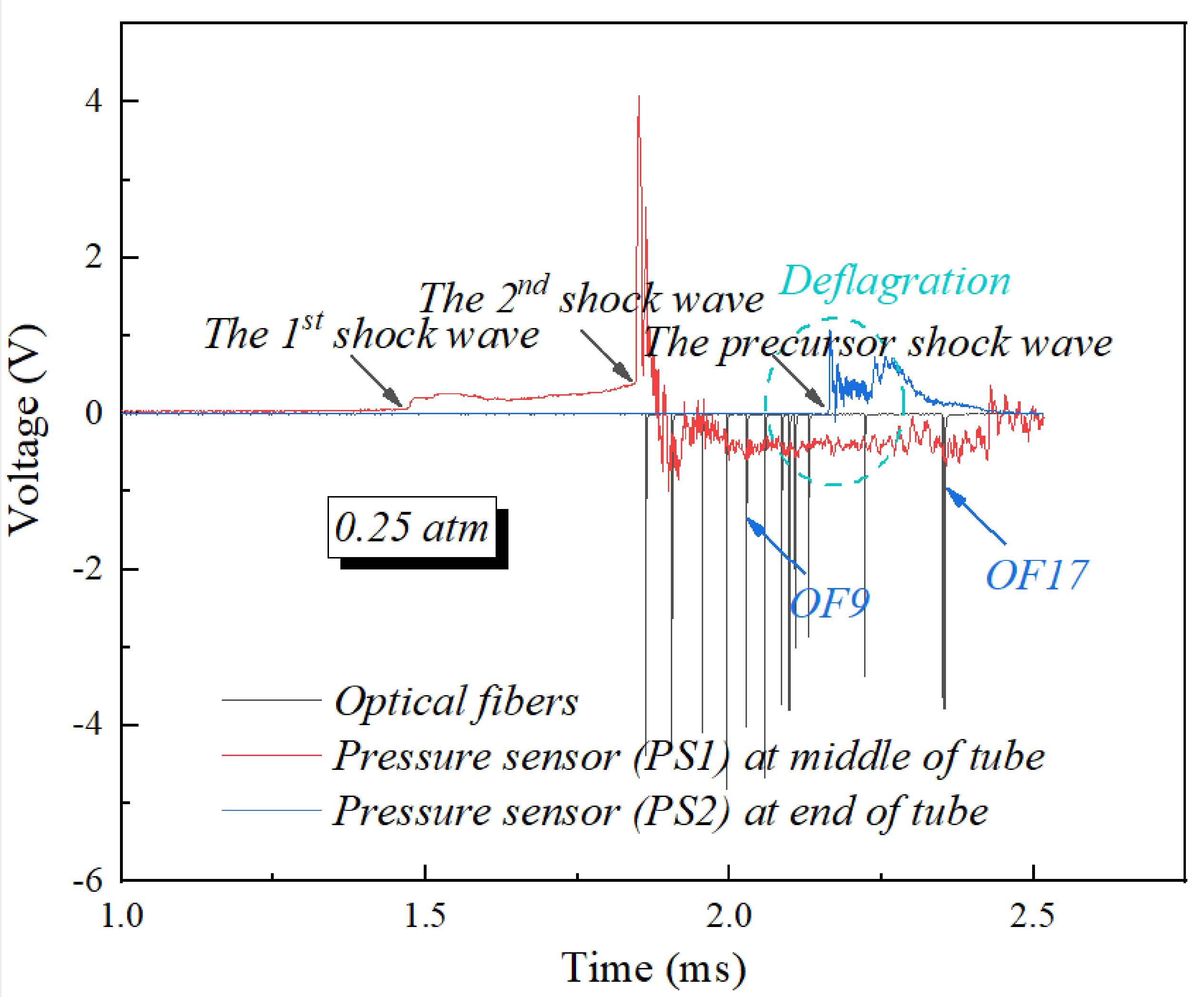
Fire and Explosion Modelling Group

Experimental Setup



Schematic diagram of the optical fibers (OF) and the PCB pressure sensors (PS) distribution.

Flame and shock wave



The signals of the overpressure and optical fibers at different P_0 with the equivalence ratio of 1.5.

1st and 2 nd shock waves also observed by in previous tests (ambient conditions)

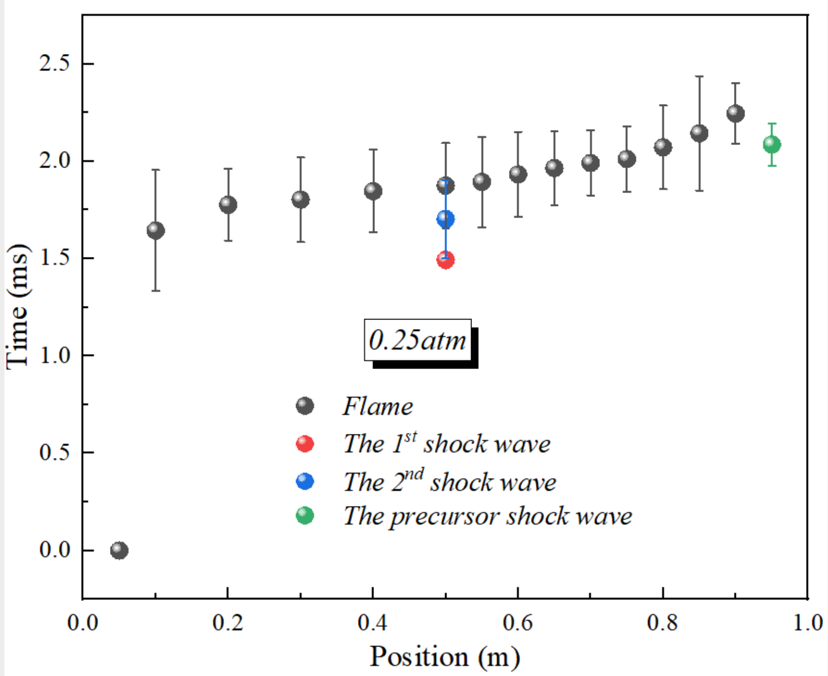
Kellenberger and Ciccarelli (2018)

Cheng et al.(2021)

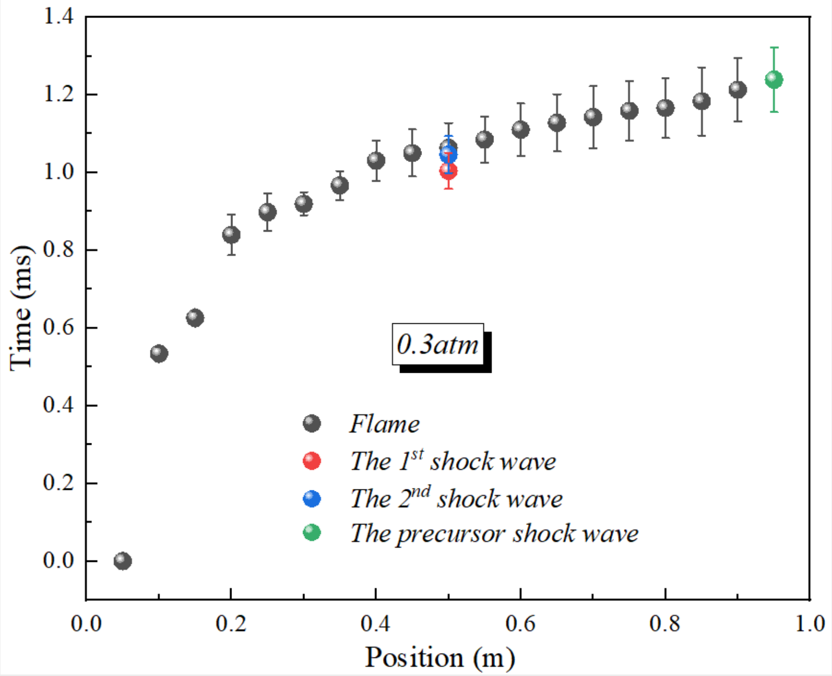
Fire and Explosion Modelling Group

Flame and shock wave

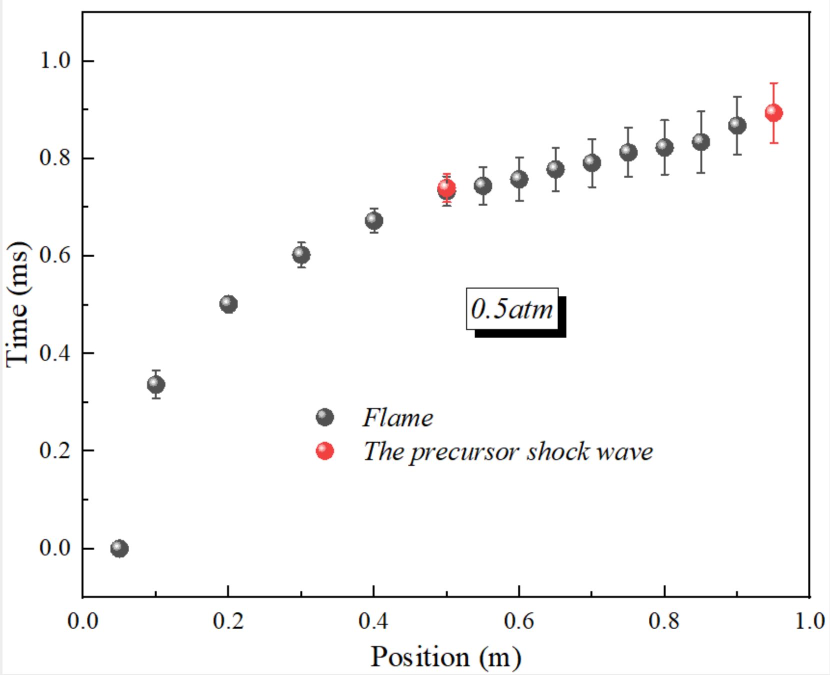
0.25 atm



0.3 atm



0.5 atm

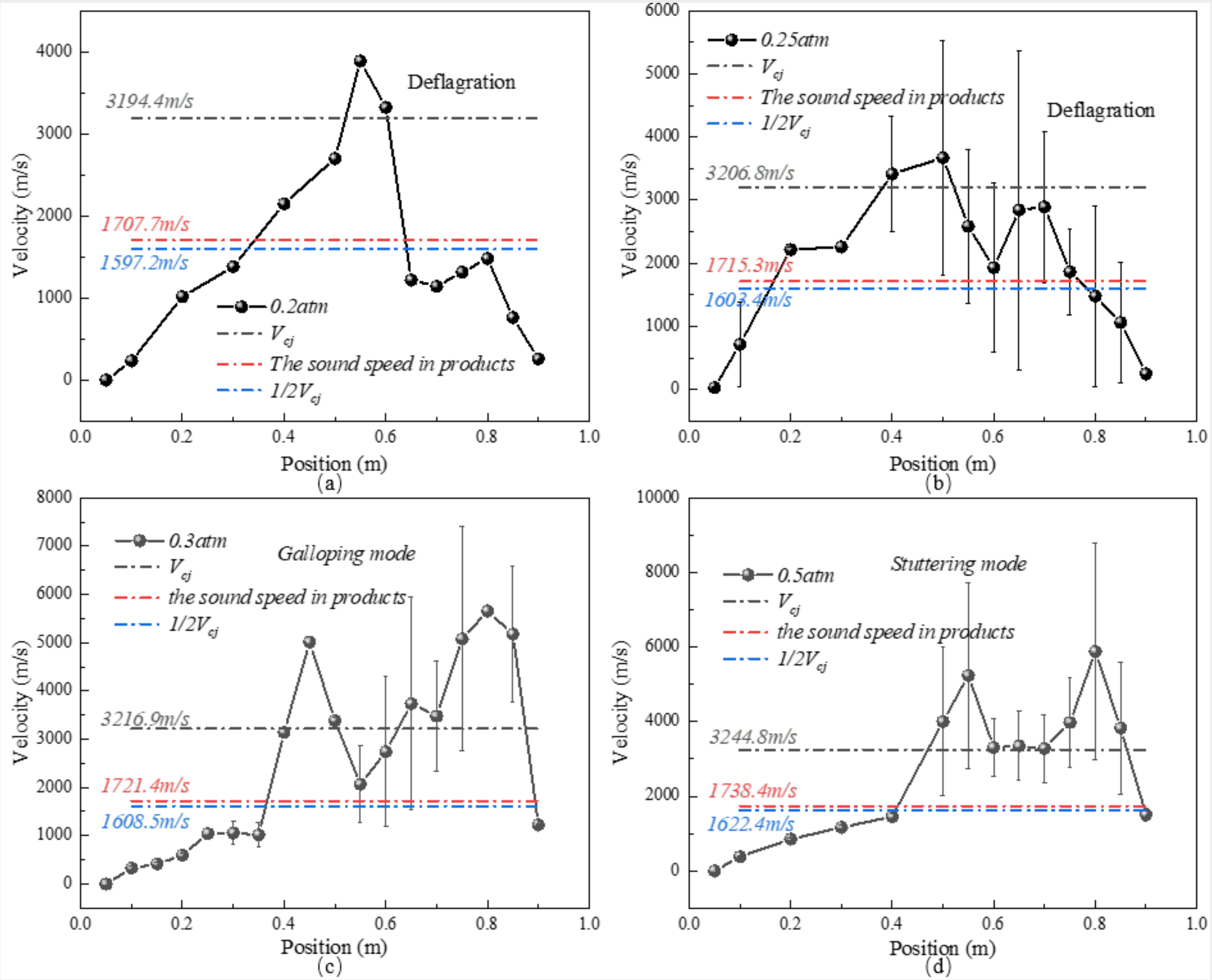


The positions of shock waves and flame versus corresponding time instants at different P_0 and 77 K with the equivalence ratio of 1.5.

Strong FA and detonation limit

0.2 atm

0.25 atm



0.3 atm

0.5 atm

The flame velocity versus position at different P_0 and 77 K with equivalence ratio of 1.5.

Strong FA

Following Dorofeev, S.B. (2007):

$$\frac{\sigma^2\beta^2(\beta/2-1)^n e^{1-\beta/2}}{6Le^n\Gamma_{n+1}\mu}=1$$

$$\frac{\sigma^2\beta^2(\beta/2-1)^n e^{1-\beta/2}}{6Le^n\Gamma_{n+1}\mu}<1$$ The quenching effect, weak FA

$$\frac{\sigma^2\beta^2(\beta/2-1)^n e^{1-\beta/2}}{6Le^n\Gamma_{n+1}\mu}>1$$ The re-ignition effect, strong FA

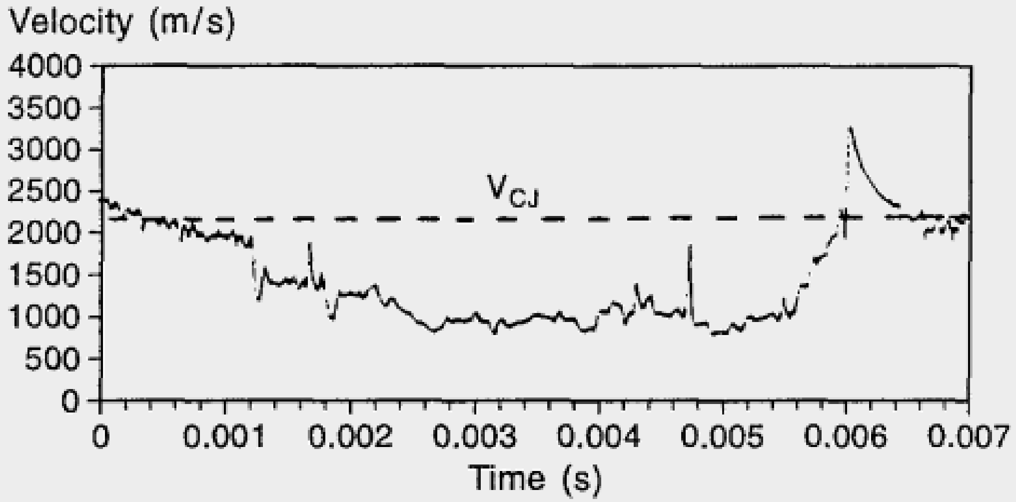
Dorofeev, S., Thermal quenching and re-ignition of mixed pockets of reactants and products in gas explosions. Proceedings of the Combustion Institute, 2007. 31(2).

The calculated values at different initial pressures

P_0 (atm), 77 K	$\frac{\sigma^2\beta^2(\beta/2-1)^n e^{1-\beta/2}}{6Le^n\Gamma_{n+1}\mu}$
0.20	13.546
0.25	14.552
0.30	15.559
0.50	19.865

Fire and Explosion Modelling Group

Detonation limit



The galloping (limiting) mode (Lee et al., 1995).

Radulescu and co-workers (2003, 2013) linked the **stability parameter** χ with the cellular structure regularity of detonation.

$$\chi_1 = \frac{t_i}{t_e}\frac{E_a}{RT_{vn}}$$

$\chi_1 > 10$ → Unstable mixture

$\chi_1 < 10$ → Stable mixture

The galloping mode is mainly observed in unstable mixtures near the limiting condition.

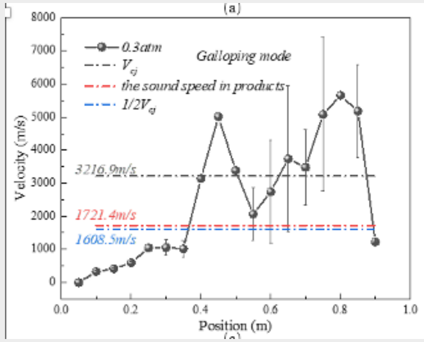
1. Lee, J., et al., Doppler interferometry study of unstable detonations. Shock Waves, 1995. 5(3): p. 175-181.
2. M.I. Radulescu, The propagation and failure mechanism of gaseous detonations: experiments in porous-walled tubes, Ph.D. Thesis, McGill University (2003)
3. J. Tang, M.I. Radulescu, Dynamics of shock induced ignition in Fickett's model: Influence of χ, Proc. Combust. Inst. 34 (2) (2013) 2035-41.

Detonation limit

The calculated results of χ_1 parameter at 77 K with the equivalence ratio of 1.5.

P_0 (atm)	t_i/t_e	E_a/RT_s	χ_1
0.20	9.521	7.954	75.728
0.25	8.684	7.434	64.559
0.30	8.986	8.154	73.270
0.50	9.457	9.887	93.498

The Galloping mode is observed at 0.3 atm.



Heat loss effect

Rubtsov (2000, 2005):

$$\frac{D^2}{2(k^2-1)} = Q - \frac{C_P R T_s^2 H_{loss} e^{E_a/RT_s}}{Q E_a}$$

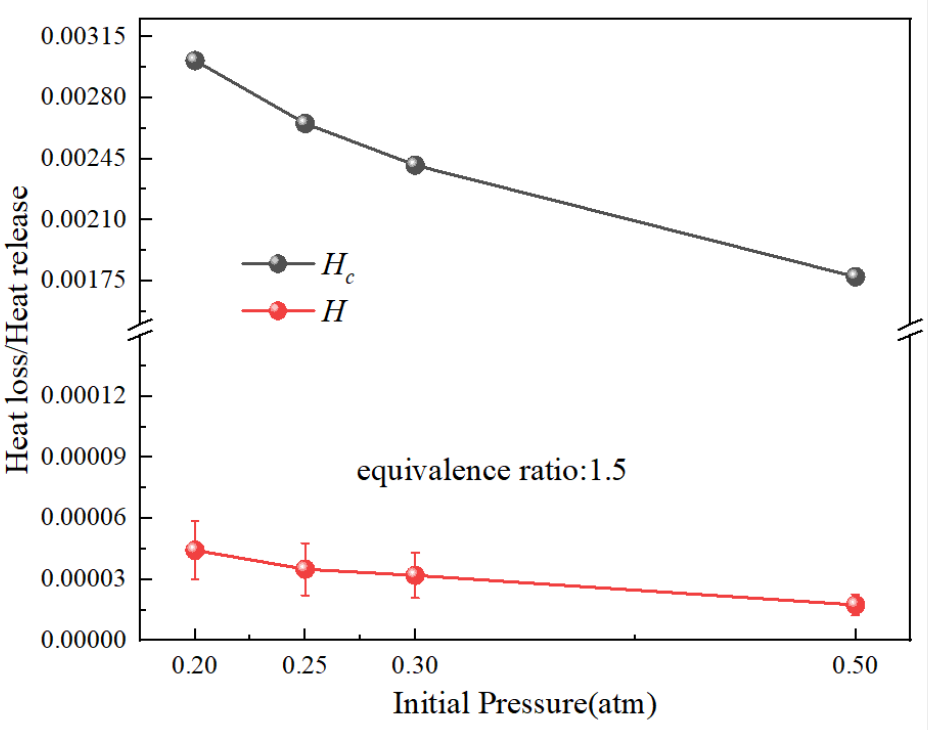
$$k/(k-1) = C_p/R$$

$$\mu = 2E_a C_p/R[1-(k-1)^2/(k+1)^2]$$

$$T_s = D^2[1-(k-1)^2/(k+1)^2]/C_p$$

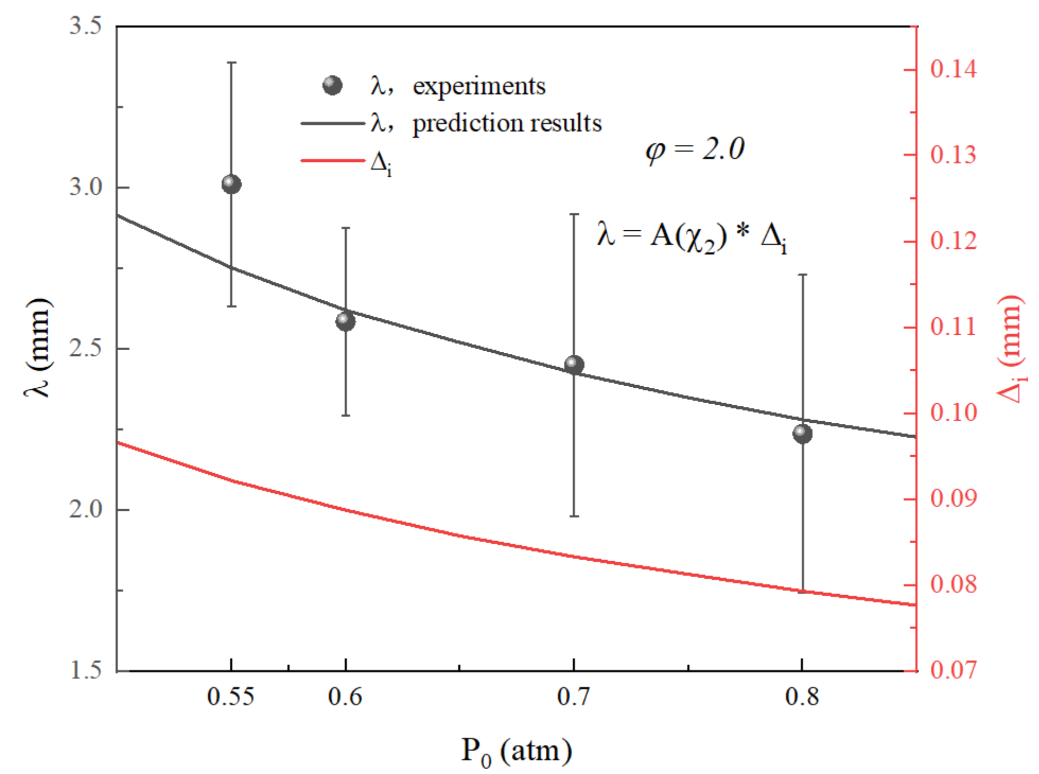
$$H_c = H_{loss}/Q$$

N.M. Rubtsov, *Effect of chemically active additives on the velocity of detonation waves and on the limit of gaseous detonation, Mendeleev Communications 10 (2000).*
N. Rubtsov, *Effect of chemically active additives on the detonation wave velocity and detonation limit in rich mixtures, Theoretical Foundations of Chemical Engineering 39 (2005).*



The ratio of heat loss to heat release as function of initial pressure at 77 K with equivalence ratio of 1.5.

Detonation cell prediction

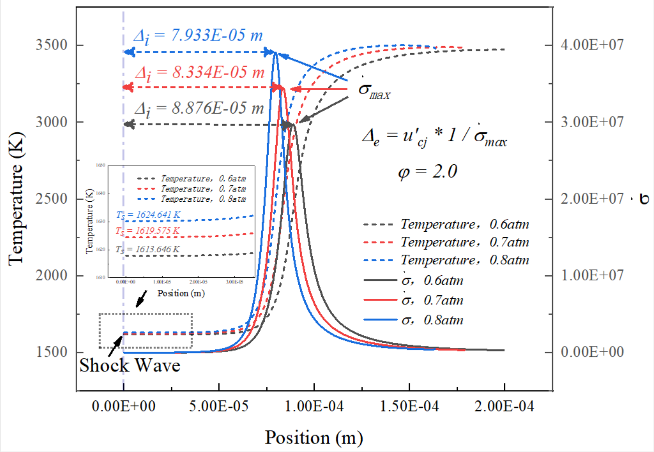


The experimental and predicted results of detonation cell width at different initial pressures and 77 K with the equivalence ratio of 2.0.

Ng et al. (2009) described the variation of the coefficient A via considering the detonation instability effect.

$$\lambda = A(\chi_2) \cdot \Delta_i = [A_0 + (a_N/\chi_2{}^N + \cdots a_1/\chi_2 + b_1\chi_2 + \cdots b_N\chi_2{}^N)] \cdot \Delta_i$$

$$\chi_2 = \frac{\Delta_i}{\Delta_e}\frac{E_a}{RT_s} = \Delta_i \frac{\dot{\sigma}_{max}}{u'_{cj}}\frac{E_a}{RT_s}$$



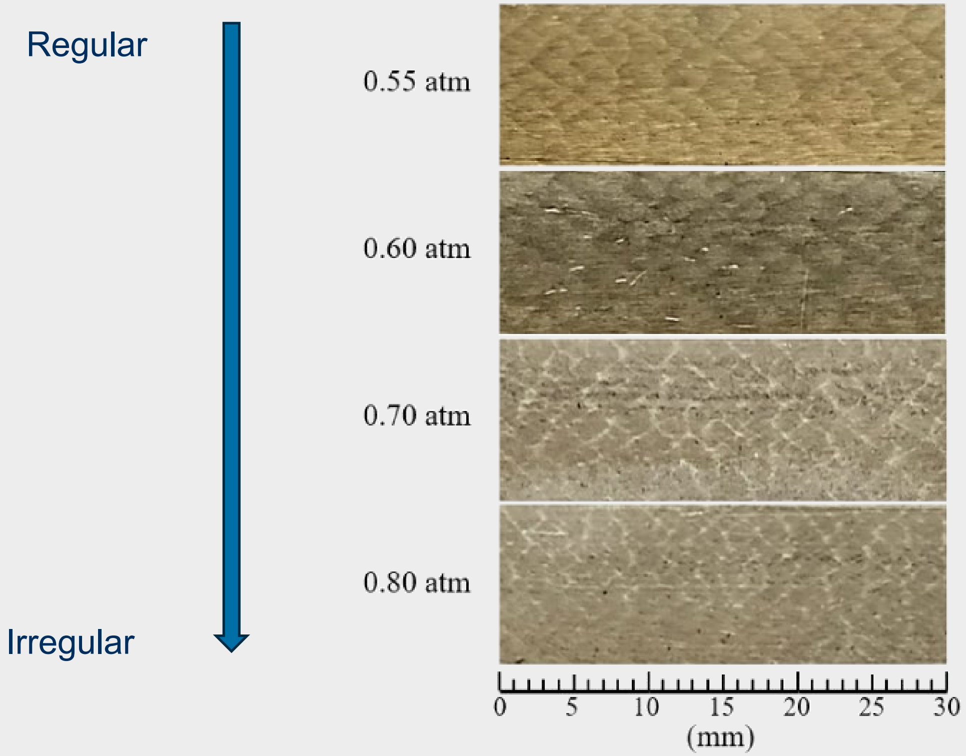
The 1-D ZND detonation profiles at 0.6-0.8 atm with the equivalence ratio of 2.0.

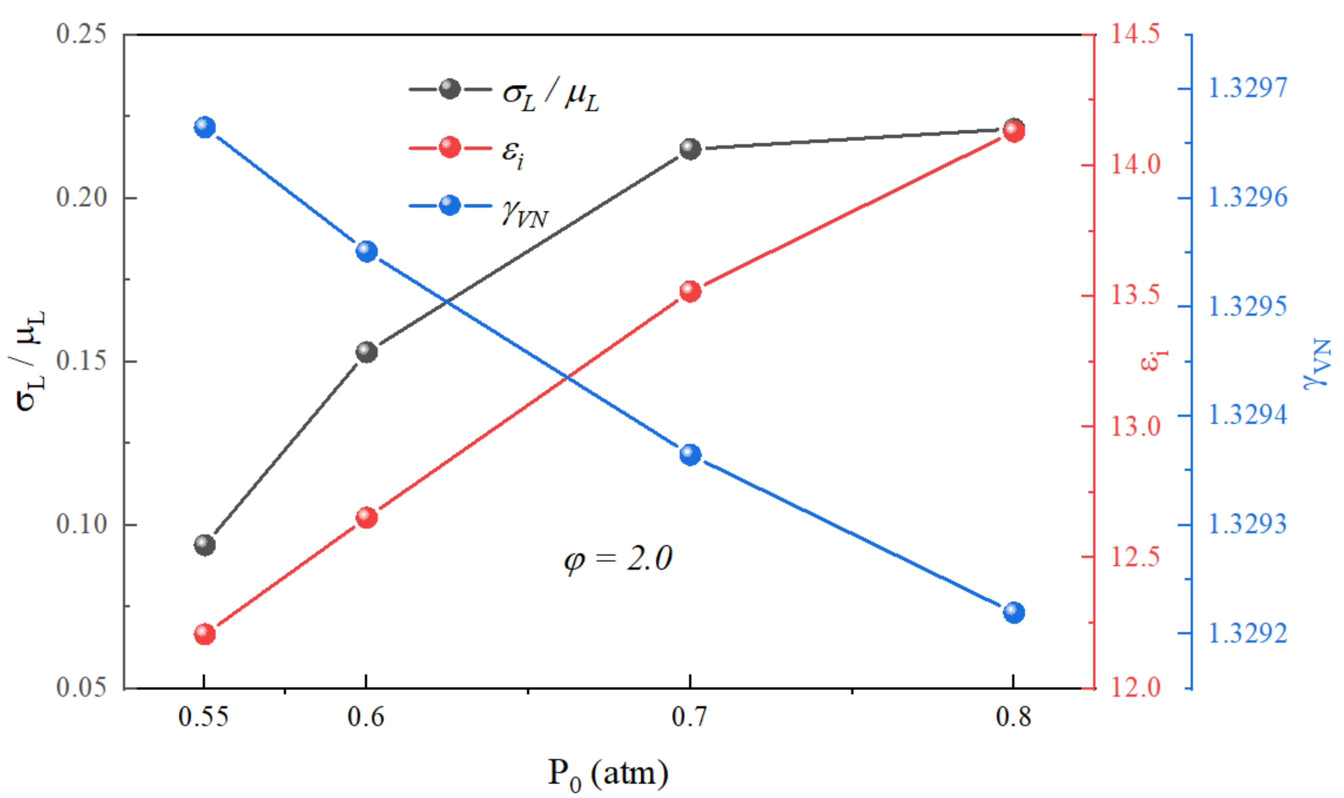
The increase in initial pressure could result in the increase in the post-shock temperature (T_s) which causes the shorter induction length and the lower maximum thermicity $\dot{\sigma}_{max}$.

H.D. Ng, J. Chao, T. Yatsufusa, J.H. Lee, Measurement and chemical kinetic prediction of detonation sensitivity and cellular structure characteristics in dimethyl ether–oxygen mixtures, Fuel 88 (2009) 124-131.

Fire and Explosion Modelling Group

Detonation cell regularity





The measured smoked foils (a) and the parameter σ_L/μ_L (b) at different initial pressures and 77 K with the equivalence ratio of 2.0.

Meagher et al. (2022): Post-shock specific heat ratio γ_{VN}, Normalized activation energy

P.A. Meagher, X. Shi, J.P. Santos, N.K. Muraleedharan, J. Crane, A.Y. Poludnenko, H. Wang, X. Zhao, Isolating gasdynamic and chemical effects on the detonation cellular structure: A combined experimental and computational study, Proc.Combus Institute, doi:10.1016/j.proci.2022.08.001(2022).

Fire and Explosion Modelling Group

Conclusions

- The strong FA caused by sufficiently larger expansion ratio were observed.
- As the initial pressure decreased from 0.50 atm to 0.20 atm with the equivalence ratio of 1.5, the processes went from stuttering, galloping and deflagration.
- The detonation limit for the considered configuration estimated to be between 0.25 atm to 0.30 atm.
- The heat loss effect on detonation limit is much smaller than the critical value to hinder transition to detonation.
- The decreases in initial pressure will cause the larger γ_{VN} and the lower ε_i which all lead to the regular detonation cell structure.

Transition to detonation in semi-confined or open conditions at cryogenic temperatures?

Acknowledgement

- Dr Xiaobo Shen is funded by EU Marie Curie Fellowship HyGAS 891173.

- The experiments were supported by the National Natural Science Foundation of China (Grant No. 22078095 and 51604121) and the Shanghai Science and Technology Committee (Grant No. 20dz1200903 and 21QC1400400).

Fire and Explosion Modelling Group