NONLINEAR ANALYSES FOR THE DYNAMICS OF SHOCK FRONTS AND DETONATIONS IN GASES

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Detonations = combustion supersonic waves

inert shock followed by an exothermal reaction zone

in gas at ordinary conditions: 1800-3400 m/s, 15-30 bar, 2500-3700 K

Old scientific topic

Recent understanding (nonlinear analyses)

Safety: explosions, nuclear power plant,..

Future propulsion: rotating detonation engines

Astrophysics: explosion of stars, supernovae I

Background in compressible fluids Planar shock waves and detonations 1860-1940



$$\begin{array}{c|c} \mathcal{D} > a_u \\ \hline \\ u_N = \mathcal{D} - v_p \\ \hline \\ Supersonic \\ \hline \\ \text{thickness: few mean free paths} \end{array}$$

Poisson 1808, Stokes 1848, Riemann 1860, Rankine 1869, Hugoniot 1889, Rayleigh 1910

1-D compressible fluids u(x,t)



Burgers equation



OVERDRIVEN DETONATION REACTING GAS

PISTON SUPORTED SUPERSONIC WAVE



Abel 1870, Berthelot et Vielle 1881, Mallard et Le Chatelier 1881, Mikhel'son 1893, Chapman 1899, Jouguet 1904,

Vielle 1900, Zel'dovich 1940, von Neumann 1942, Döring 1943,



Cellular structure of the front of the detonation waves experiments & numerics 1960-2017

Cellular structure of the detonation wave

Shchelkin and Troshin 1960



Front view



Markings left on soot-coated foils at the wall of the tube

Triple points



2-D Regular structure

Triple point = 2-D singularity of a shock front



example of a triple point propagating in a uniform flow



B.Maxwell, R.Bhattacharjee, S. Lau-Chapelaine, S.Falle, G. Sharpe and M. Radulescu to appear in *Journal of Fluid Mechanics* 2017

 $CH_4 + 2O_2$ $p = 3.5kP_a$ 2D geometry experiment



High activation energy: Irregular structure and transient phenomena



Successive frames $11\mu s$ apart

B.Maxwell, R.Bhattacharjee, S. Lau-Chapelaine, S.Falle, G. Sharpe and M. Radulescu to appear in *Journal of Fluid Mechanics* 2017 $CH_4 + 2O_2$ $p = 3.5kP_a$

Turbulent mixing of unburnt and burnt pockets?



B.Maxwell, R.Bhattacharjee, S. Lau-Chapelaine, S.Falle, G. Sharpe and M. Radulescu

to appear in Journal of Fluid Mechanics 2017

 $CH_4 + 2O_2 \quad p = 3.5kP_a$



Numerical simulation

Experiment

Theoretical analyses of cellular structures 1996-2017



1st step: one-dimensional instability 1996-2002

1-D compressible, inviscid and reactive gas mixture



3 nonlinear modes: Entropy wave + 2 acoustic waves

too complicated system for a general analytical solution

1-D longitudinal oscillation of the ZND structure



Analytical solutions have been obtained in two limiting cases (opposite conditions):

Strongly overdriven detonati	on in the Newtonian limit	(P.C. & L. He 1996)
quasi-isobaric flow		
dominant mechanism:	entropy wave \longrightarrow	

CJ (or near CJ) conditions close to the instability threshold (P.C. & F.A. Williams 2002) transonic flow dominant mechanism: acoustic wave

Overdriven detonation



Relative distance

Rankine-Hugoniot relations

detonation velocity shocked gas temperature

 $\mathcal{D} \Leftrightarrow T_N$

large activation energy

 $\beta \equiv E/k_b T_N \gg 1$

large sensitivity of the distribution of reaction rate to temperature

steady state: $\Omega(\Theta_N, \mathbf{x})$

$$\Theta_N \equiv \beta \frac{(T_N - \overline{T}_N)}{\overline{T}_N} = O(1)$$

$$\begin{array}{c|ccc} M_{u} \equiv \mathcal{D}/a_{u} & M_{N} \equiv u_{N}/a_{N} \\ \hline & \text{initial fluid} \\ \hline & \mathcal{D} > a_{u} \\ \hline & & \\ \hline & & \\ \hline & & \\ M_{u} > 1 \\ (p_{u}, \rho_{u}) \end{array} & \begin{array}{c} \text{M}_{N} \equiv u_{N}/a_{N} \\ \text{shocked fluid, Neumann state} \\ u_{N} < a_{N} \\ \hline & & \\ M_{N} < 1 \\ (p_{N}, \rho_{N}) \end{array} & \begin{array}{c} M_{N}^{2} = \frac{(\gamma - 1)M_{u}^{2} + 2}{2\gamma M_{u}^{2} - (\gamma - 1)} \\ M_{N}^{2} = \frac{(\gamma - 1)M_{u}^{2} + 2}{2\gamma M_{u}^{2} - (\gamma - 1)} \\ \gamma \equiv c_{p}/c_{V} \end{array}$$

strongly overdriven detonations in the Newtonian limit (P.C. & L. He 1996)

$$\epsilon^2 \equiv \frac{1}{M_u^2} \ll 1 \qquad (\gamma - 1) = O(\epsilon^2)$$

 $M_N = O(\epsilon)$

shocked gas: quasi-isobaric approximation

Rankine-Hugoniot

low Mach number: $M_N \ll 1$

$$\frac{|\delta p_N|}{\rho_N a_N |\dot{\alpha}_t|} = O(M_N), \quad \delta u_N \approx \dot{\alpha}_t \Rightarrow \frac{|\delta p_N|}{\rho_N a_N |\delta u_N|} = O(M_N)$$

negligible pressure effects; acoustic waves quasi-instantaneous

strongly overdriven detonations in the Newtonian limit

quasi-isobaric approximation in the shocked gases



strongly overdriven detonations in the Newtonian limit quasi-isobaric approximation in the shocked gas



OK with DNS



formation of singularities propagating in the transverse direction

Nonlinear dynamics of inert shock fronts

P. Clavin, Journal of Fluid Mechanics (2013)

B. Denet, K. Biamo, G. Lodato, L. Vervisch and P. Clavin, Combust. Sci. Technol. (2014)

G. Lodato, L. Vervisch and P. Clavin, Journal of Fluid Mechanics (2016)

P. Clavin, Combust. Sci. Technol. (2017)



Result for a polytropic gas :

Oscillatory mode with a non-radiating condition of the acoustic wave



Strong shock in the Newtonian limit

$$\epsilon^2 \equiv \frac{1}{M_u^2} \ll 1 \qquad (\gamma - 1) = O(\epsilon^2)$$

$$M_N^2 = O(\epsilon^2)$$



$$\epsilon^2 \equiv \frac{1}{M_u^2} \ll 1 \qquad (\gamma - 1) = O(\epsilon^2)$$

quasi-isobaric approximation



$$\epsilon^{2} \equiv \frac{1}{M_{u}^{2}} \ll 1 \quad (\gamma - 1) = O(\epsilon^{2}) \implies M_{N} = O(\epsilon) \qquad \underbrace{\mathcal{D} > a_{u}}_{M_{u} > 1} \qquad \underbrace{\mathcal{D} > a_{u}}_{M_{N} < 1}$$

Order of magnitude of the cell size



markings left on sooted coil foils at the wall trajectory of triple points



Secondary

Heat

point

Propagation

pure (inert) shock wave

Mach stems propagating in the transverse direction



What is a Mach stem ?

Triple point = 3 shock waves + 1 slip line (degenerescence of shear layer) called also contact line discontinuity (Courant Friedrichs 1948)

steady triple points were first observed as a reflexion of an oblique incident shock at a wall







example of a triple point propagating in a uniform flow

Spontaneous formation of Mach stems on shock fronts

Shock reflection from a wavy wall

2-D Direct Numerical Simulation

Lodato et al. J.F.M (2016)





Denet et al. C.S.T (2015)

Structure similar to that of cellular detonation



Formation of singularities. Simple transverse wave: Burgers equation for $\alpha'_{y}(y,t)$

Formation of a singularity in a finite time

$$\frac{\partial^2 \alpha}{\partial t^2} - \overline{a}_N^2 \frac{\partial^2 \alpha}{\partial y^2} + \mathcal{D} \frac{\partial}{\partial t} \left(\frac{\partial \alpha}{\partial y}\right)^2 = 0$$

Burgers equation for $\alpha_y'(y,t) \equiv \partial \alpha / \partial y$ along a simple transverse wave

$$\left[\frac{\partial}{\partial t} \pm \overline{a}_N \frac{\partial}{\partial y}\right] \alpha'_y + 2\mathcal{D}\left(\alpha'_y \frac{\partial}{\partial y} \alpha'_y\right) = 0$$

Geometrical construction



nonlinear term \Rightarrow Collapse of points C and D by a Huygens construction

shear wave degenerates \Rightarrow slip line

acoustic wave degenerates \Rightarrow secondary shock

$$\frac{\partial^2 \alpha}{\partial t^2} - \overline{a}_N^2 \frac{\partial^2 \alpha}{\partial y^2} + \overline{\mathcal{D}} \frac{\partial}{\partial t} \left(\frac{\partial \alpha}{\partial y} \right)^2 = 0$$

Numerical solution with an ondulated initial condition

Comparison with DNS







Model equation

Interaction between a strong shock and a weak vortex



Extension to 3-D: Shock turbulence interaction

$$x = \alpha(y, z, t) \qquad \mathbf{u}_e(x, y, z, t) = (u_e, v_e, w_e) \qquad |\mathbf{u}_e|/a_u < \overline{a}_N/\mathcal{D} \ll 1$$
$$\frac{\partial^2 \alpha}{\partial t^2} - \overline{a}_N^2 \bigtriangleup \alpha + \mathcal{D} \frac{\partial}{\partial t} |\nabla \alpha|^2 = 2 \frac{\overline{a}_N}{\mathcal{D}} \frac{\mathrm{d}}{\mathrm{d}t} u_e(-\mathcal{D}t, y, z, t) \qquad \overline{a}_N/a_u = O(1)$$

Turbulence length-scale at the shock

Shock surface after a while





The size and the amplitude of the cells increase with the time



Nonlinear dynamics of cellular detonations

P. Clavin and R. Daou, J. Fluid. Mech. (2002)
P. Clavin and B. Denet, Phys. Rev. Lett. (2002)
P. Clavin and F.A. Williams, Phil. Trans. R. Soc. (2012)
P. Clavin and G. Searby, Cambridge Univ. Press (2016)
P. Clavin, Combust. Sci. Technol. (2017)

Nonlinear theory for the cellular structure



Weakly nonlinear analysis at the instability threshold

transverse instability > longitudinal instability \Rightarrow small heat release

Analytical solutions have been obtained in the Newtonian approximation for two limiting cases (opposite conditions) :



Weakly nonlinear analysis of the cellular patterns of strongly overdriven detonations near the stability limit in the Newtonian limit

$$M_N \ll 1 \qquad \qquad q_N \equiv \frac{q_m}{c_p \overline{T}_N} \ll 1$$

- Poincaré-Adronov (Hopf) bifurcation at small heat release $q_N = O(M_N^2)$

Non zero and finite wavelength and frequency: $\Lambda \approx d_N/M_N$ $\omega \approx 2\pi/t_N$ $d_N \equiv \overline{u}_N \tau_N$ $t_N \equiv \tau_{reac}(T_N)$

- Result: nonlinear equation for the detonation front

Non-dimensional form $(\alpha(y,t) \text{ scaled with } d_N, y \text{ scaled with } d_N/M_N, t \text{ scaled with } t_N)$ NL term linear terms due to combustion $\frac{\partial^2 \alpha}{\partial t^2} - \frac{\partial^2 \alpha}{\partial y^2} + \frac{\partial}{\partial t} \left(\frac{\partial \alpha}{\partial y}\right)^2 = [q_N G(\alpha) - M_N \sqrt{q_N} D(\alpha)]$ linear growth linear damping (quasi-isobaric mechanism) (compressible effect) $x = \alpha(y,t)$ $x = \alpha(y,t)$ $\alpha(y,t) = \tilde{\alpha}e^{iky+\sigma t}$ $Re[\sigma(k)]$ $Im[\sigma(k_c)] \neq 0$ $M_N \ll 1 \qquad q_N = O(M_N^2)$



Long time selection

Good qualitative agreement with the experimental observation



selected wavelength > most linearly unstable wavelength



Extensions

3-D geometry
$$x = A(y, z, t)$$
 $\nabla^2 \equiv \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$
linear instability acoustic stabilisation
 $\frac{\partial^2 A}{\partial t^2} - c^2 \nabla^2 A + \frac{\partial |\nabla A|^2}{\partial t} = \mathbf{q}_N L^{(i)}(A) - 2\overline{M}_N \sqrt{q_N} \frac{\partial}{\partial t} L^{(a)}(A) \quad \overline{M}_N \ll 1 \quad q_N = O(\overline{M}_N^2)$
 $L^{(i)}(\alpha) = \frac{\beta_N(\gamma - 1)l_{\beta_N}^{(i)}(A)}{P_N(\alpha)} + l_q^{(i)}(A) \quad \left\{ \begin{array}{c} l_{\beta_N}^{(i)}(A) = \frac{\partial^2}{\partial t^2} \int_0^\infty \Omega'_N(x)A(y, z, t - x)dx, & 1-\text{D instability} \\ l_q^{(i)}(\alpha) = \nabla^2 \int_0^\infty \Psi(x)A(y, z, t - x)/dx & 3-\text{D instability} \end{array} \right\}$

Secondary bifurcation: crossing the threshold of the planar instability $\beta_N(\gamma - 1)q_N$



Conclusion

Most of the complex phenomena of the cellular detonations in gases have been deciphered by nonlinear analytical studies

Amongst the phenomena that are still not fully understood is the deflagration to detonation transition, a problem of importance for safety reason and also for the explosion of supernovae I

Another open problem is the fate of the strong shock formed during the gravitational collapse of the iron core of a massive stars at the end of their life (supernovae II)



Cambridge University Press 2016