Turbulence generation by planar detonations in heterogeneous mixtures

Workshop on Fluid Dynamics 2019

A- Cuadra-Lara*, C. Huete & M. Vera

*acuadra@ing.uc3m.es

Group of Fluid Mechanics
Universidad Carlos III de Madrid

Granada, Spain | July 23, 2019

uc3m | Universidad Carlos III de Madrid

Outline

Detonation Turbulence Phenomena

Description of the problem

- 1D Reactive Rankine-Hugoniot relation
- Effect of local perturbations in the fuel mass fraction
- Qualitative analysis

Mathematical model

- Non-dimensional governing equations
- Linearized Reactive Rankine-Hugoniot Equations
- Problem domain and boundary conditions

Ongoing & Parallel work

References

Useful stuff

Here we are dealing with two diferent phenomena which are, independently, very complex to model: Detonations & Turbulence.

Therefore, strong simplifications must be done in order to get an analytically tractable problem

- **Detonation:** planar and stable.
- **Turbulence:** weak, homogeneous and isotropic[1].

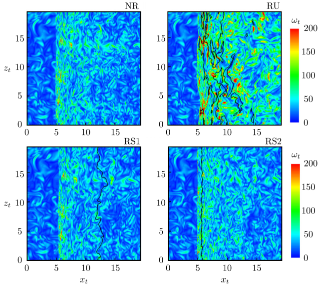


Figure 1: Instantaneous vorticity patterns for NR, RU, RS1, and RS2 obtained at the cut plane $y_t = (6.61\pi)/2$. Black contour lines on the reactive cases correspond to the isolines of nearly complete depletion of reactant $Y = 0.01$ (Huete 2017).

[1] G. Keith Batchelor. The theory of homogeneous turbulence. Cambridge university press, 1953.

uc3m

Definitions

- density:

$$\rho = \rho_o \left(1 + W\hat{Y}\right), \qquad (1)$$

- heat release:

$$q = q_o \left(1 + H\hat{Y}\right), \qquad (2)$$

- mixture ratio:

$$W = \frac{1 - \frac{W_{air}}{W_{fuel}}}{Y_{fuel} + \frac{W_{air}}{W_{fuel}}\left(1 - Y_{fuel}\right)}. \qquad (3)$$

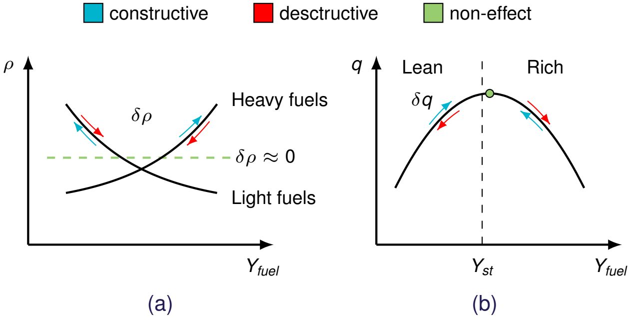


Figure 2: Variation of mixture density (a) and heat release (b) with the fuel mass fraction and the equivalence ratio.

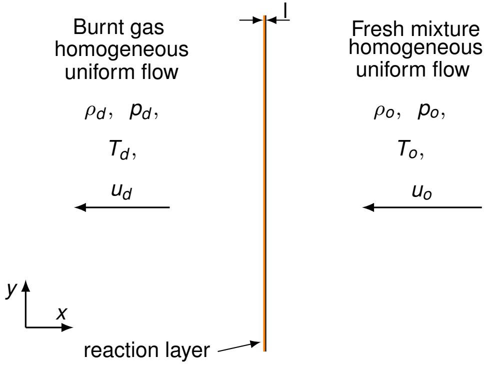
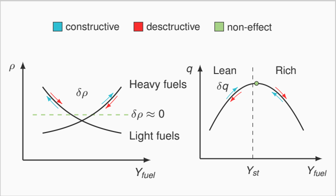


Figure 3: Sketch of the planar detonation front, where l is the thickness of the reaction layer. Reference frame moving with the shock surface.

Description of the problem
1D Reactive Rankine-Hugoniot relation

$$\frac{p_d}{p_o} = \frac{(\gamma+1)\rho_d - (\gamma-1)\rho_o + 2(\gamma-1)\rho_d\rho_o q/p_o}{(\gamma+1)\rho_o - (\gamma-1)\rho_d}$$



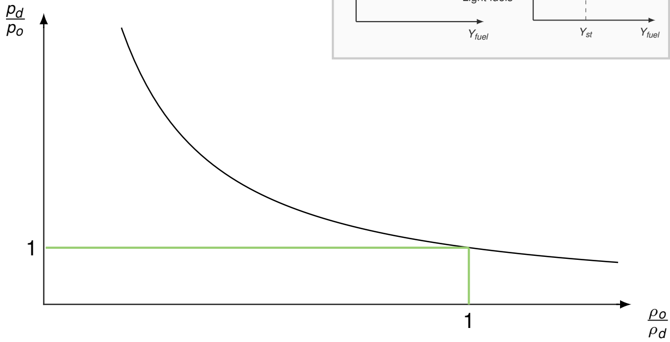
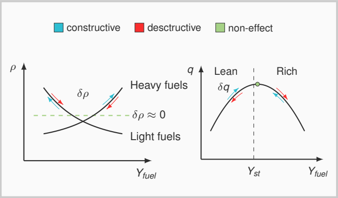


Figure 4: Perturbations on the Rankine-Hugoniot relation.

Description of the problem

1D Reactive Rankine-Hugoniot relation



$$\frac{p_d}{p_o} = \frac{(\gamma+1)\rho_d - (\gamma-1)\rho_o + 2(\gamma-1)\rho_d\rho_o q/p_o}{(\gamma+1)\rho_o - (\gamma-1)\rho_d}$$

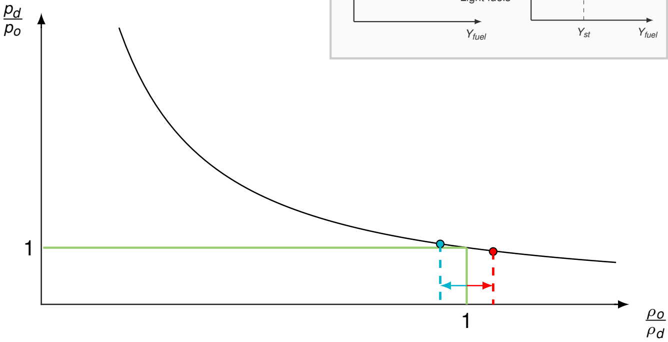
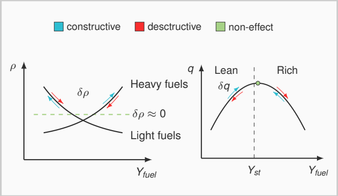


Figure 4: Perturbations on the Rankine-Hugoniot relation.

$$\frac{p_d}{p_o} = \frac{(\gamma+1)\rho_d-(\gamma-1)\rho_o+2(\gamma-1)\rho_d\rho_o q/p_o}{(\gamma+1)\rho_o-(\gamma-1)\rho_d}$$



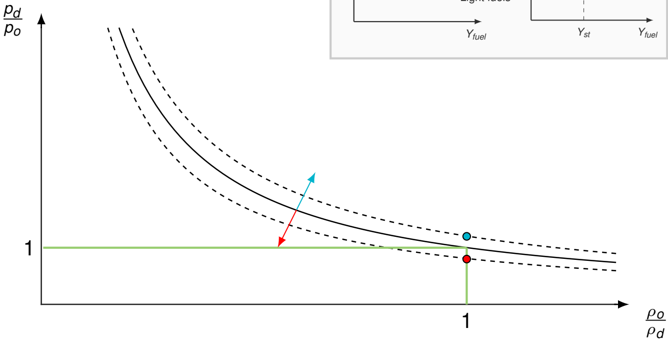
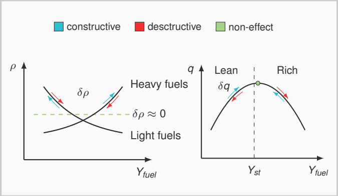


Figure 4: Perturbations on the Rankine-Hugoniot relation.

$$\frac{p_d}{p_o} = \frac{(\gamma+1)\rho_d - (\gamma-1)\rho_o + 2(\gamma-1)\rho_d\rho_o q/p_o}{(\gamma+1)\rho_o - (\gamma-1)\rho_d}$$



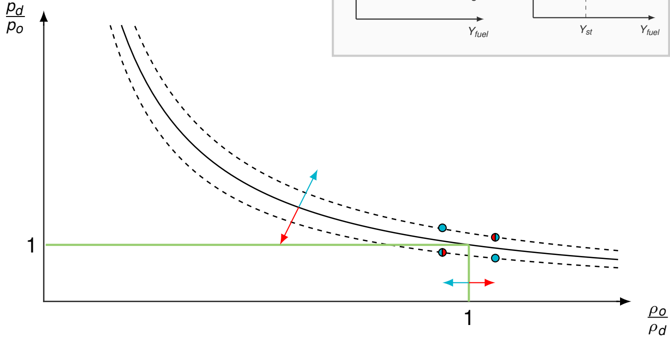


Figure 4: Perturbations on the Rankine-Hugoniot relation.

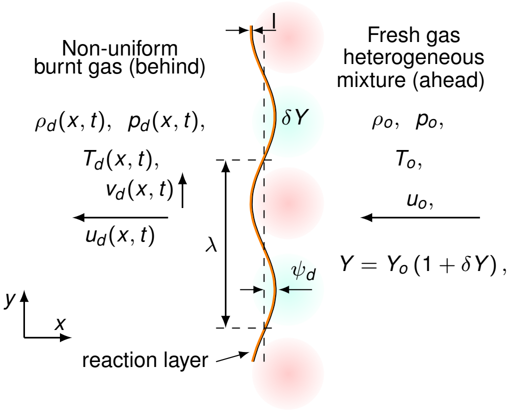


Figure 5: Sketch of the corrugated detonation front, where ψ_d is the amplitude of the detonation shape deviations respect to the planar shape, and must satisfy $l \ll \psi_{d0} \ll \lambda$. Reference frame moving with the shock surface.

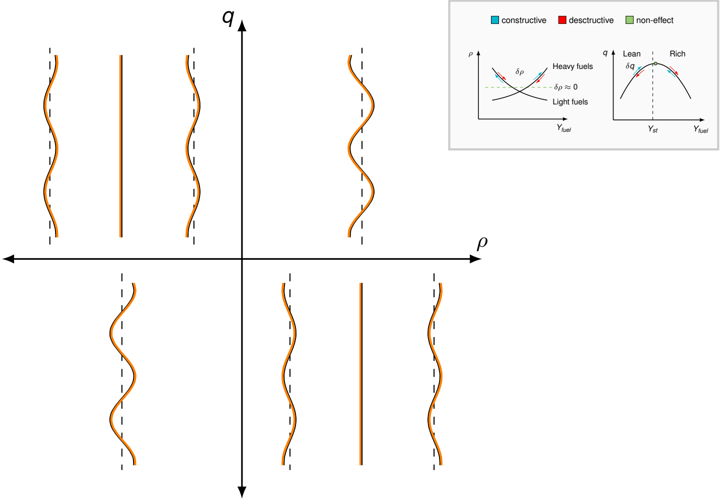


Figure 6: Qualitative analysis between the heat release and the mixture density.

Mathematical model
Assumptions

- Perfect gases.

- Perfect gases.
- Thin detonation limit: **The detonation wave is treated as a pure discontinuity**[2]. Infinitely fast chemistry, $Da \gg 1$ in order to satisfy $l \ll \xi$.

[2] C. Huete *et al.* Physics of Fluids, 25:076105,2013.

- Perfect gases.
- Thin detonation limit: **The detonation wave is treated as a pure discontinuity**[2]. Infinitely fast chemistry, $Da \gg 1$ in order to satisfy $l \ll \xi$.
- Thick detonation limit: The size of the perturbations is much smaller than the detonation thickness[3]. **Linear theory,** $\dot{\xi} \ll \lambda$.

[2] C. Huete *et al.* Physics of Fluids, 25:076105,2013.
[3] C. Huete *et al.* Physics of Fluids, 26:116101, 2014.

- Perfect gases.
- Thin detonation limit: **The detonation wave is treated as a pure discontinuity**[2]. Infinitely fast chemistry, $Da \gg 1$ in order to satisfy $l \ll \xi$.
- Thick detonation limit: The size of the perturbations is much smaller than the detonation thickness[3]. **Linear theory,** $\dot{\xi} \ll \lambda$.
- Isotropic probability density function (**analysis of all the spectrum**).

[2] C. Huete *et al.* Physics of Fluids, 25:076105,2013.
[3] C. Huete *et al.* Physics of Fluids, 26:116101, 2014.

- Perfect gases.
- Thin detonation limit: **The detonation wave is treated as a pure discontinuity**[2]. Infinitely fast chemistry, $Da \gg 1$ in order to satisfy $l \ll \xi$.
- Thick detonation limit: The size of the perturbations is much smaller than the detonation thickness[3]. **Linear theory,** $\dot{\xi} \ll \lambda$.
- Isotropic probability density function (**analysis of all the spectrum**).

The functions of interest are perturbed, namely

$$\hat{p}(\hat{x},\tau) = \hat{p}_a(\hat{x},\tau) = \mathbb{P} e^{i(\hat{\omega}\tau - \hat{k}\hat{x})} e^{i\hat{y}}, \tag{4}$$

$$\hat{\rho}(\hat{x},\tau) = \hat{\rho}_a + \hat{\rho}_e, \tag{5}$$

$$\hat{u}(\hat{x},\tau) = \hat{u}_a + \hat{u}_r, \tag{6}$$

$$\hat{v}(\hat{x},\tau) = \hat{v}_a + \hat{v}_r, \tag{7}$$

for the pressure, density, longitudinal velocity and transverse velocity, respectively.

[2] C. Huete *et al.* Physics of Fluids, 25:076105,2013.

[3] C. Huete *et al.* Physics of Fluids, 26:116101, 2014.

Non-dimensional compressible Euler equations:

$$\frac{\partial \hat{\rho}}{\partial \tau} + \frac{\partial \hat{u}}{\partial \hat{x}} + \frac{\partial \hat{v}}{\partial \hat{y}} = 0, \tag{8a}$$

$$\frac{\partial \hat{u}}{\partial \tau} + \frac{\partial \hat{p}}{\partial \hat{x}} = 0, \tag{8b}$$

$$\frac{\partial \hat{v}}{\partial \tau} + \frac{\partial \hat{p}}{\partial \hat{y}} = 0, \tag{8c}$$

$$\frac{\partial \hat{p}}{\partial \tau} - \frac{\partial \hat{\rho}}{\partial \tau} = 0, \tag{8d}$$

can be linearly manipulated to give:

$$\frac{\partial^2 \hat{p}}{\partial \tau^2} = \frac{\partial^2 \hat{p}}{\partial \hat{x}^2} + \frac{\partial^2 \hat{p}}{\partial \hat{y}^2}. \tag{9}$$

Non-dimensional compressible Euler equations + periodically symmetric condition:

$$\frac{\partial \hat{\rho}}{\partial \tau} + \frac{\partial \hat{u}}{\partial \hat{x}} + \hat{v} = 0, \tag{8a}$$

$$\frac{\partial \hat{u}}{\partial \tau} + \frac{\partial \hat{p}}{\partial \hat{x}} = 0, \tag{8b}$$

$$\frac{\partial \hat{v}}{\partial \tau} - \hat{p} = 0, \tag{8c}$$

$$\frac{\partial \hat{p}}{\partial \tau} - \frac{\partial \hat{\rho}}{\partial \tau} = 0, \tag{8d}$$

Two-dimensional periodically symmetric wave equation for the burnt gas:

$$\frac{\partial^2 \hat{p}}{\partial \tau^2} = \frac{\partial^2 \hat{p}}{\partial \hat{x}^2} - \hat{p}. \tag{9}$$

The perturbations **behind the shock** (one of the boundary conditions) are given by the linearized Rankine Hugoniot equations

$$\frac{D\xi_d}{D\tau} = \frac{R_d}{R_d - 1}\left[\frac{1+\Gamma_d}{2M_d}\hat{p}_d + \frac{M_d}{2}\left(W(2-R_d) - \Delta_d\right)\frac{M_d}{2}\hat{Y}\right], \tag{10a}$$

$$\hat{u}_d = \frac{1+\Gamma_d}{2M_d}\hat{p}_d + \frac{M_d}{2}\left(\Delta_d - R_d W\right)\hat{Y}, \tag{10b}$$

$$\hat{v}_d = M_d(R_d - 1)\frac{\partial \xi_d}{\partial \hat{y}}, \tag{10c}$$

$$\hat{\rho}_d = \frac{\Gamma_d}{M_d^2}\hat{p}_d + \Delta_d\hat{Y}, \tag{10d}$$

where ξ_d is the dimensionless shock ripple amplitude, and Γ_d and Δ_d are the Rankine-Hugoniot slope and the heat release contribution, both downstream, respectively.

Combining RH-equations with conservation equations we get:

$$a_1 \frac{\partial^2 \hat{p}_d}{\partial \tau^2} + a_2 \frac{\partial^2 \hat{p}_d}{\partial \tau \partial \hat{x}} + a_3 \frac{\partial^2 \hat{p}_d}{\partial \hat{x}^2} + a_4 \frac{\partial^2 \hat{p}_d}{\partial \hat{y}^2} = f(\hat{\omega_s}), \tag{11}$$

where a_1, a_2, a_3, and a_4 are constants, and $f(\hat{\omega_s})$ is a function that depends of the shock frequency.

Combining RH-equations with conservation equations we get:

$$a_1 \frac{\partial^2 \hat{p}_d}{\partial \tau^2} + a_2 \frac{\partial^2 \hat{p}_d}{\partial \tau \partial \hat{x}} + a_3 \frac{\partial^2 \hat{p}_d}{\partial \hat{x}^2} + a_4 \frac{\partial^2 \hat{p}_d}{\partial \hat{y}^2} = f(\hat{\omega_s}), \qquad (11)$$

where a_1, a_2, a_3, and a_4 are constants, and $f(\hat{\omega_s})$ is a function that depends of the shock frequency.
Assuming

$$\hat{p} = \mathbb{P} e^{i(\hat{\omega}\tau - \hat{k}\hat{x})}, \qquad (12)$$

which satisfy the wave equation (9), and in order to apply normal modes

$$\hat{Y}_s = e^{i(\hat{\omega_s}\tau + \hat{y})}, \qquad (13)$$

which gives

$$\hat{\omega}^2 = \hat{k}^2 + 1, \qquad (14)$$

$$\hat{\omega_s} = \hat{\omega} - \hat{k} M_d, \qquad (15)$$

where $\hat{\omega}$ and $\hat{\omega_s}$ are the dimensionless frequency and the dimensionless shock frequency, respectively.

Mathematical model
Linearized Rankine-Hugoniot Equations

Dispersion relation:

$$\left[-\hat{\omega}_s^2\sigma_b - \hat{\omega}_s\sqrt{\hat{\omega}_s^2 + M_d^2 - 1} - M_d^2\left(R_d - 1\right)\sigma_a\right]\mathbb{P}e^{i(\hat{\omega}_s\tau)} = f(\hat{\omega}_s)e^{i\hat{\omega}_s\tau}, \quad (16)$$

Dispersion relation:

$$\left[-\hat{\omega}_s^2\sigma_b - \hat{\omega}_s\sqrt{\hat{\omega}_s^2 + M_d^2 - 1} - M_d^2\left(R_d - 1\right)\sigma_a\right]\mathbb{P}e^{i(\hat{\omega}_s\tau)} = f(\hat{\omega}_s)e^{i\hat{\omega}_s\tau}, \quad (16)$$

$$\left[\zeta\sigma_b + \zeta\sqrt{\zeta^2 - 1}\left(1 - M_d^2\right)^{-1/2} - \sigma_c\right]\mathbb{P}e^{i\hat{\omega}_s\tau} = f^*(\hat{\omega}_s)e^{i\hat{\omega}_s\tau}, \quad (17)$$

with

$$\zeta = \frac{\hat{\omega}_s}{\sqrt{1 - M_d^2}}. \quad (18)$$

Dispersion relation:

$$\left[-\hat{\omega}_s^2\sigma_b - \hat{\omega}_s\sqrt{\hat{\omega}_s^2 + M_d^2 - 1} - M_d^2\left(R_d - 1\right)\sigma_a\right]\mathbb{P}e^{i(\hat{\omega}_s\tau)} = f(\hat{\omega}_s)e^{i\hat{\omega}_s\tau}, \quad (16)$$

$$\left[\zeta\sigma_b + \zeta\sqrt{\zeta^2 - 1}\left(1 - M_d^2\right)^{-1/2} - \sigma_c\right]\mathbb{P}e^{i\hat{\omega}_s\tau} = f^*(\hat{\omega}_s)e^{i\hat{\omega}_s\tau}, \quad (17)$$

with

$$\zeta = \frac{\hat{\omega}_s}{\sqrt{1 - M_d^2}}. \quad (18)$$

- $\zeta > 1$:

$$\mathbb{P} = \frac{f^*(\hat{\omega}_s)}{\zeta\sigma_b + \zeta\sqrt{\zeta^2 - 1}\left(1 - M_d^2\right)^{-1/2} - \sigma_c}. \quad (19)$$

Dispersion relation:

$$\left[-\hat{\omega}_s^2\sigma_b - \hat{\omega}_s\sqrt{\hat{\omega}_s^2 + M_d^2 - 1} - M_d^2\left(R_d - 1\right)\sigma_a\right]\mathbb{P}e^{i(\hat{\omega}_s\tau)} = f(\hat{\omega}_s)e^{i\hat{\omega}_s\tau}, \quad (16)$$

$$\left[\zeta\sigma_b + \zeta\sqrt{\zeta^2 - 1}\left(1 - M_d^2\right)^{-1/2} - \sigma_c\right]\mathbb{P}e^{i\hat{\omega}_s\tau} = f^*(\hat{\omega}_s)e^{i\hat{\omega}_s\tau}, \quad (17)$$

with

$$\zeta = \frac{\hat{\omega}_s}{\sqrt{1 - M_d^2}}. \quad (18)$$

- $\zeta > 1$:

$$\mathbb{P} = \frac{f^*(\hat{\omega}_s)}{\zeta\sigma_b + \zeta\sqrt{\zeta^2 - 1}\left(1 - M_d^2\right)^{-1/2} - \sigma_c}. \quad (19)$$

- $\zeta < 1$:

$$\mathrm{Re}\left\{\mathbb{P}e^{i\hat{\omega}_s\tau}\right\} = a\,cos(\hat{\omega}_s\tau) + sin(\hat{\omega}_s\tau). \quad (20)$$

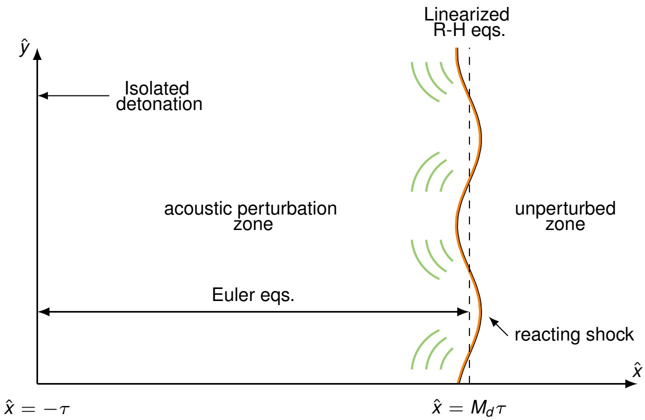
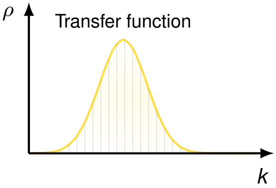


Figure 7: Problem domain and boundary conditions. Reference frame moving with the burnt gas.

Ongoing work

- Downstream averages (Velikovich, 2012). Superposition of the modes (linear theory).



- Characterize the turbulence generated by a given dispersion relationship in the heterogenous mixture.
- Evaluate how the propagation velocity and average values downstream are affected with respect to the homogenous case.
- Multiphase (droplets and high energy materials).

Parallel work

Development and validation of a new MATLAB®/GUI based thermochemical code, A. Cuadra-Lara & M. Vera.

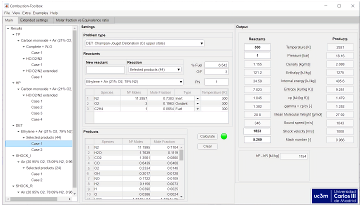
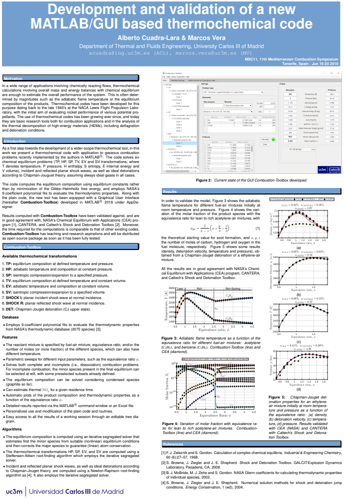


Figure 8: Current state of the GUI Combustion-Toolbox developed.



References

[1] Lee, J. The Detonation Phenomenon. Cambridge University Press (2008).

[2] Kailasanath, K. Review of propulsion applications of detonation waves. AIAA journal 38.9 (2000): 1698-1708.

[3] Veyssiere, B., and B. A. Khasainov. Structure and multiplicity of detonation regimes in heterogeneous hybrid mixtures. Shock Waves 4.4 (1995): 171-186.

[4] Kailasanath, K. Liquid-fueled detonations in tubes. Journal of Propulsion and Power 22.6 (2006): 1261-1268.

[5] Watanabe, Hiroaki, et al. Numerical investigation on propagation behavior of gaseous detonation in water spray. Proceedings of the Combustion Institute 37.3 (2019): 3617-3626.

[6] Velikovich, A. L., C. Huete, and J. G. Wouchuk. Effect of shock-generated turbulence on the Hugoniot jump conditions. Physical Review E 85.1 (2012): 016301.

[7] Huete, César and Jin, Tai and Martínez-Ruiz, Daniel and Luo, Kun. Interaction of a planar reacting shock wave with an isotropic turbulent vorticity field. Physical Review E, 96.5 (2017): 053104.

Thank you for your attention!

Useful stuff

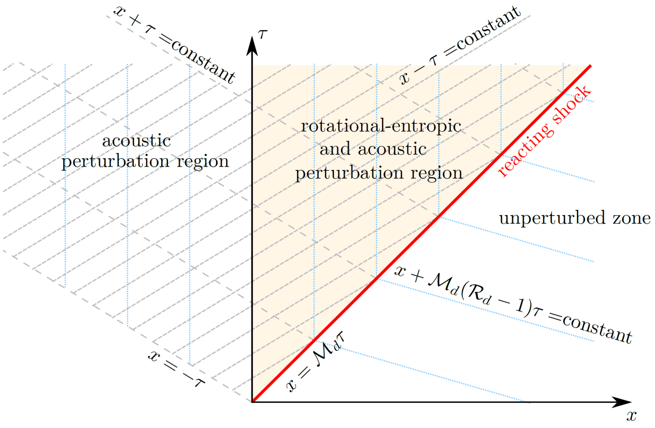


Figure 9: Integration domain and distinguished regions. Blue dotted lines refer to the particle paths, grey dashed lines indicate the positive and negative characteristic paths, respectively, and the red solid line defines the detonation trajectory (Huete 2019).