Detonation-diffuse interface interactions: failure, re-initiation and propagation limits

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Dutch Section of the Combustion Institute Webinar

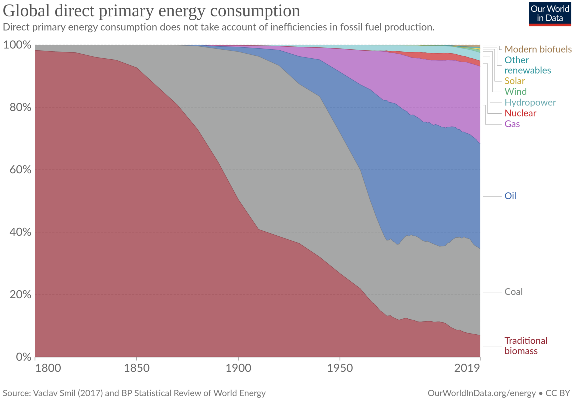
September 23, 2022

Outline

1. PART I: Context and motivation
   - Why combustion?
   - Accidental combustion events
   - Combustion 101
   - Detonation fundamentals
2. PART II: Talk
   - Non-ideal detonation propagation

Outline

Why combustion?



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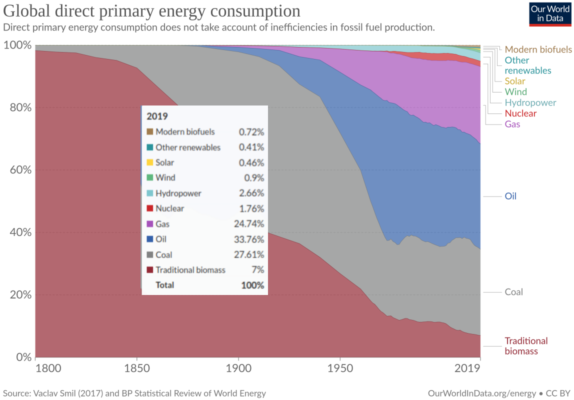

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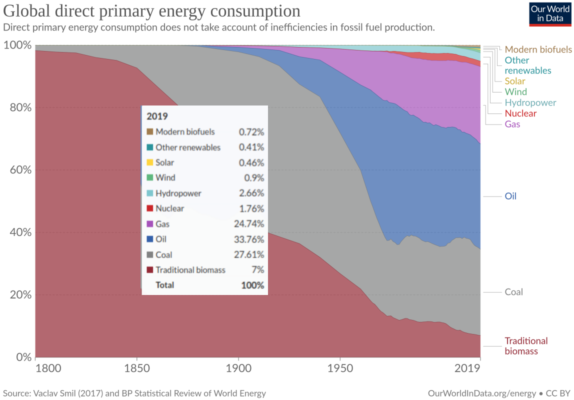

Take aways

- Over ∼ 90% comes from burning something
- Increase in renewables contained in consumption growth
- Picture unlikely to change

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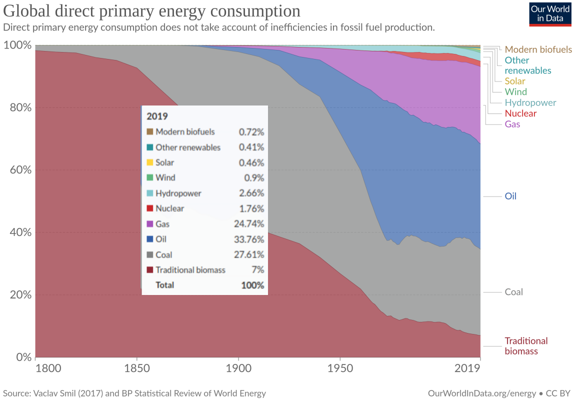

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What to do?

Push for efficiency through...

- Low-carbon bio-/H_2-enriched
- Carbon-free (i.e., H_2, NH_3)

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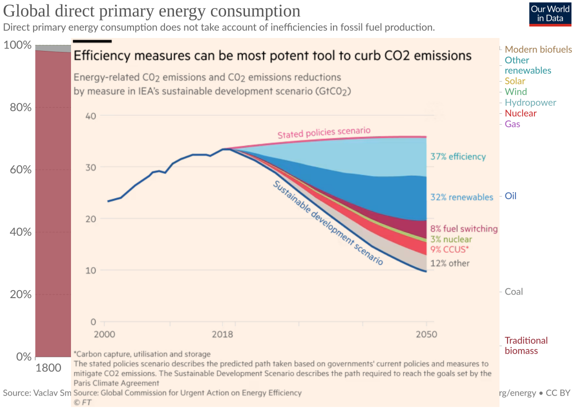

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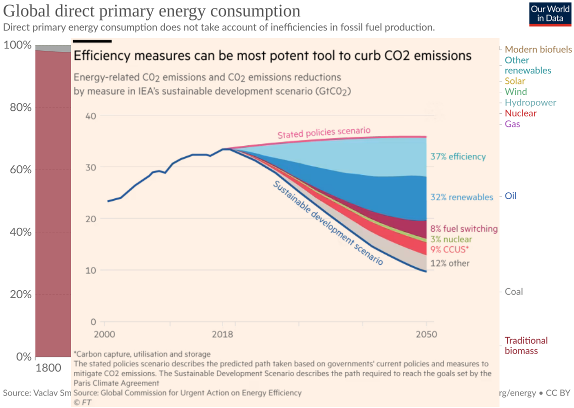

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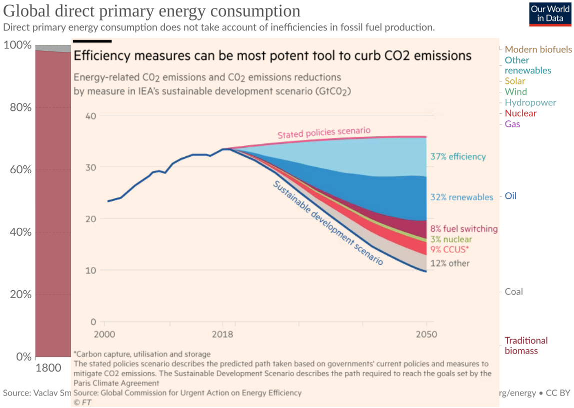
Is the future electric?

Why combustion?



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What to do?

Push for efficiency through...

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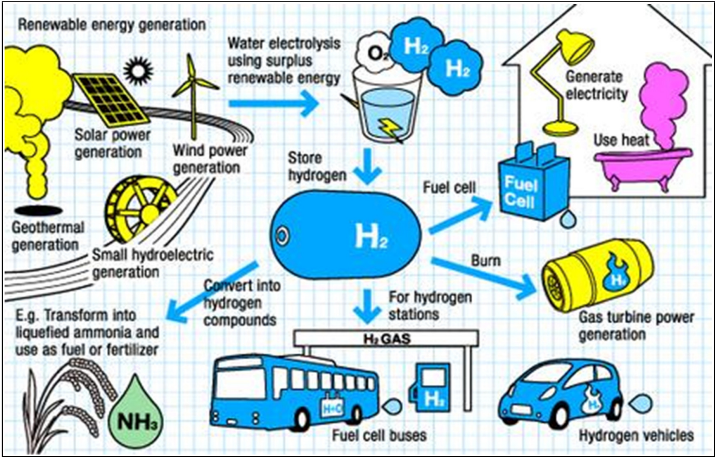
Is the future electric?

rather *eclectic*[1]

[1] *adjective.* deriving ideas, style, or taste from a broad and diverse range of sources.

Carbon-free combustion

Support the development of a **H_2 economy** to enable the global energy transition



Source : P.I. Jimenez-Calvo (2019) (Ph.D Thesis, Université de Strasbourg, FRA)

Practical aspects

Concerns with H_2?

- Wide flammability limits compared to hydrocarbons
  - In air: $\%X_{H_2,vol} \sim 4 - 75$;
    ($\%X_{C_6H_{14},vol} \sim 1.05 - 6.7$, $\%X_{C_7H_{16},vol} \sim 1.1 - 7.5$, $\%X_{Jet-A,vol} \sim 0.6 - 4.9$)
- Low ignition energy
  - In air: $H_2 \sim 0.016$ mJ @ 28%;
    (C_6H_{14} / $C_7H_{16} \sim 0.24$ mJ @ 3.4% / 3.8%)
- Light (buoyant) and highly diffusive molecule
  - Difficult to store – as a gas at $\uparrow p$ (safety); as a liquid at cryogenic conditions (expensive!)
  - Good for storage outdoors, issues with indoor storage / use (i.e. ceilings, tunnels, parking garages)

Production (electrolizers)

Storage (Composite tanks)

Handling (General public)

Accidental combustion events - safety

Aircraft

Nuclear

Chemical

Mining

Accidental combustion events - safety

Large scale destruction + losses of lives + environmental impact

Aircraft

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How to prevent these events?

Aircraft

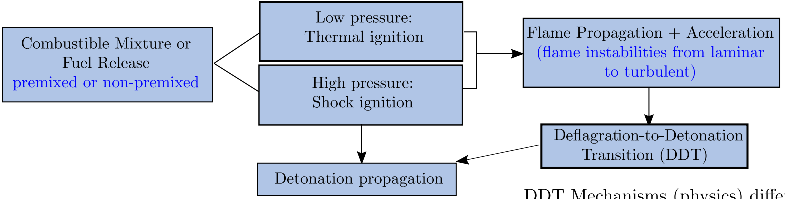
Nuclear

Chemical

Mining

Accidental combustion events - research interests (so far)

The big picture - typical accident scenario



+ Safety aspects
+ Harness high rate of energy release

DDT Mechanisms (physics) differ based on configuration

+ Smooth channels ($h \sim \mathcal{O}(\delta)$)
  - Shock induced (between shock-flame)
  - Shock-/flame-boundary layer interactions
+ Obstacle laden channels
  - Shock-induced (upon reflection from obstacles)

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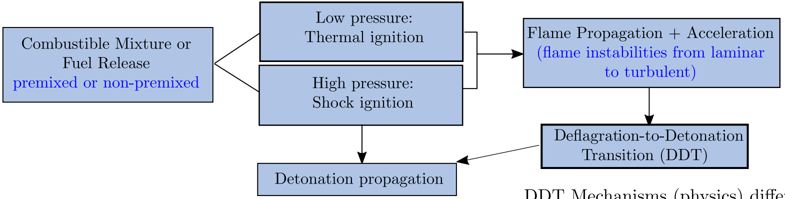

+ Safety aspects

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Courrières (1904)

Buncefield (2005)

Beyrouth (2020)

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Combustion 101 (1/4)

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But... how do we make sense of it? with Continuum Mechanics

Combustion 101 (1/4)

Reacting flow =
fluid mechanics + heat/mass transfer + thermodynamics + chemistry

But... how do we make sense of it? with Continuum Mechanics

Mathematical Description of Nature (AKA Conservation laws)

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \text{ (Mass)}$$
$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \tau \text{ (Momentum)}$$
$$\partial_t (\rho Y_k) + \nabla \cdot (\rho \mathbf{u} Y_k) = -\nabla \cdot \mathbf{j_k} + \dot{\omega}_k \text{ (Species)}$$
$$\partial_t (\rho e_t) + \nabla \cdot (\rho \mathbf{u}(e_t + p)) = -\nabla \cdot \mathbf{j_q} \text{ (Energy)}$$

with $e_t = \sum_{k=1}^{N} h_k Y_k - p/\rho + \frac{1}{2}\mathbf{u}\cdot\mathbf{u}$; $\tau = \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$

Combustion 101 (2/4)

Experimental and numerical challenges in reacting flow

Wide range of temporal and spatial scales involved

- Size of experimental aparatus - $\mathcal{O}(\text{m})$
- Hydrodynamic/thermal BL thickness - $\mathcal{O}(\mu\text{m}) - \mathcal{O}(\text{mm})$
- Chemical induction/ignition times - $\mathcal{O}(\text{s})/\mathcal{O}(\text{ms})$
- Induction length and flame thickness - $\mathcal{O}(\mu\text{m})$

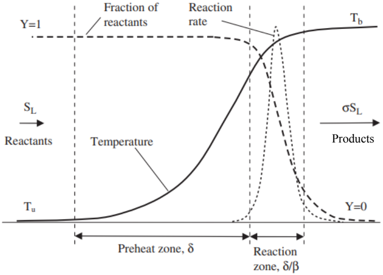
Size of detailed chemical kinetic mechanisms

- Hydrocarbons commonly used for transportation

Fuel	Reactions	Species
n-hexane (n-C_6H_{14})	2271	508
ethylene (C_2H_4)	1016	169
hydrogen (H_2)	21	9

Combustion 101 (3/4)

Deflagrations/Flames



Propagation physics

heat/mass diffusion

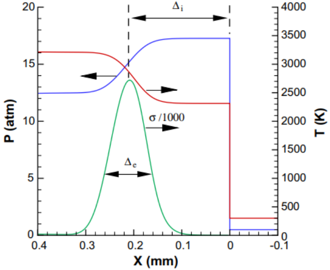
Across interface

$\rho \downarrow$, $p \sim$ cte

Steady speed

$s_L \sim \mathcal{O}$(m/s)

Detonations



Propagation physics

shock-induced ignition

Across interface

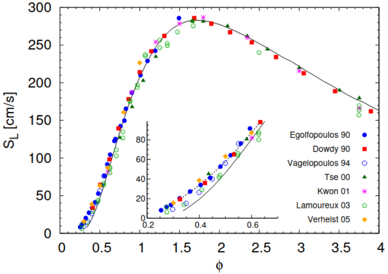
$\rho \uparrow$, p, $\uparrow$

Steady speed

$D_{\mathrm{CJ}} \sim \mathcal{O}$(km/s)

Combustion 101 (4/4)

Deflagrations/Flames



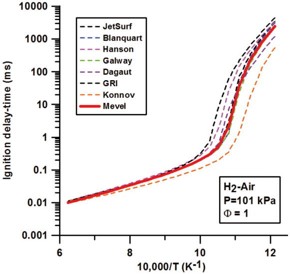
Propagation physics

heat/mass diffusion

Metric of interest

laminar burning velocity, s_L

Detonations



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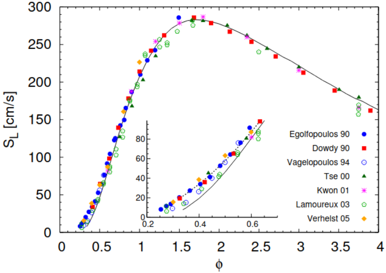
Ignition delay time, τ_{ign}

(Effective activation energy, $E_a/R_u T_{\text{ref}}$)

Combustion 101 (4/4)

Deflagrations/Flames



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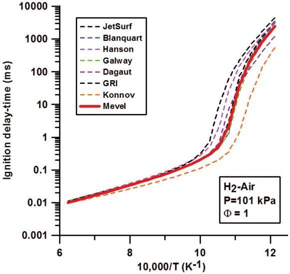

Propagation physics

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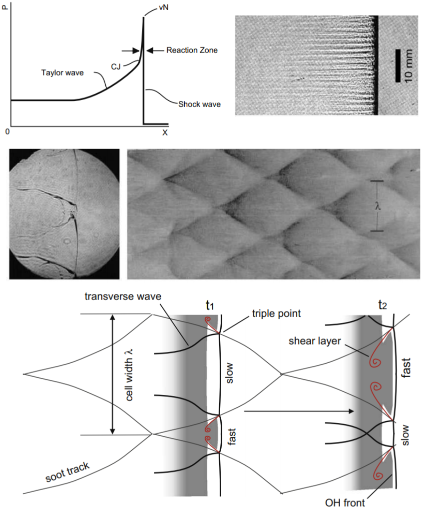
Fundamental properties - both experimentally determined

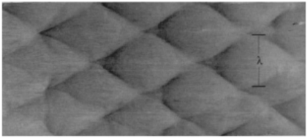
Detonation fundamentals[2] (1/4)



[2]Shepherd, J. E. (2009). Detonation in gases. Proc. Combustion Inst., 32(1), 83-98.

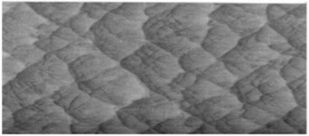
Detonation fundamentals (2/4)

λ is used to classify detonations



Regular

($\downarrow E_a/R_u T_{\mathrm{vN}}$)



Irregular

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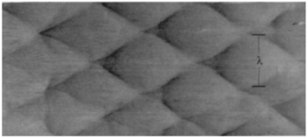

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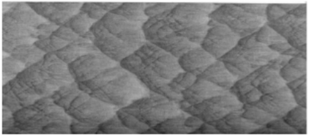

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Unless highly diluted in Ar, λ is not a single well-defined quantity!

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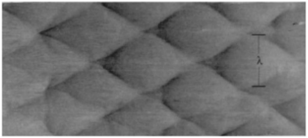

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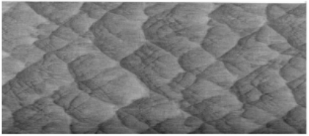


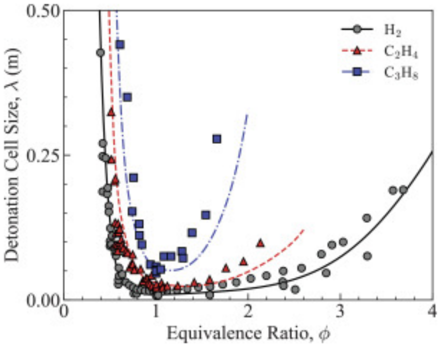
Irregular

$(\uparrow E_a/R_uT_{\mathrm{vN}})$

Unless highly diluted in Ar, λ is not a single well-defined quantity!

λ is a function of the chemistry ($E_a/R_uT_{\mathbf{vN}}$), i.e., ϕ, p_0, T_0

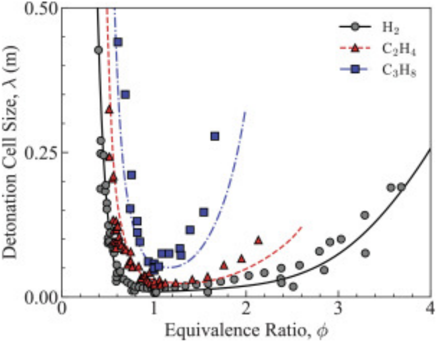
Detonation fundamentals (3/4)



Source : Bauwens, C. R. L., & Dorofeev, S. B. (2020) Combustion and Flame, 221, 338-345.

[3] $\lambda \sim 10$ mm (H_2-Air) / $\lambda \sim 300$ mm (CH_4-Air); Conditions: $p_0 = 100$ kPa and $\phi = 1$
Source: Caltech's Detonation Database

Detonation fundamentals (3/4)



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λ useful for explosion hazards & safety evaluations/engineering[3]

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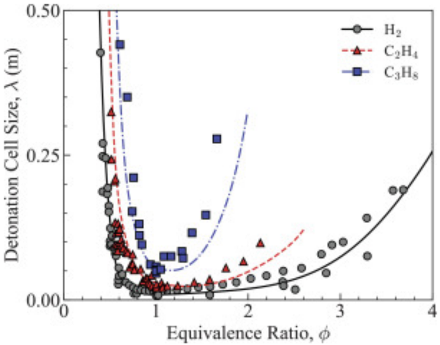

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λ useful for explosion hazards & safety evaluations/engineering[3]

Limiting behavior (propagation, transmission, re-initiation) given as $f(L/\lambda)$; L: geometrical scale

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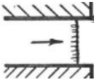
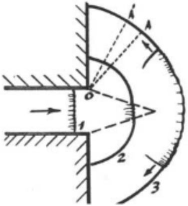
Detonation fundamentals (4/4)

Propagation/transmission limits[4]





Propagation

Tubes: $L = d \sim \lambda/\pi$

Square channels: $L = h > \lambda$

Transmission

Tubes: $L = d \sim 13\lambda$

Square channels: $L = h > 10\lambda$

[4] Caltech's Detonation Database (https://shepherd.caltech.edu/detn_db/html/db.html)

Detonation fundamentals (4/4)

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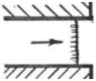
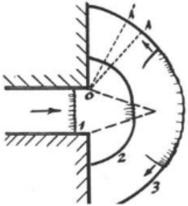




Propagation

Tubes: $L = d \sim \lambda/\pi$

Square channels: $L = h > \lambda$

Transmission

Tubes: $L = d \sim 13\lambda$

Square channels: $L = h > 10\lambda$

Depends on mixture type *regular* vs. *irregular* and BCs

(Reported values as high as 40λ and as low as 3λ)

[4] Caltech's Detonation Database (https://shepherd.caltech.edu/detn_db/html/db.html)

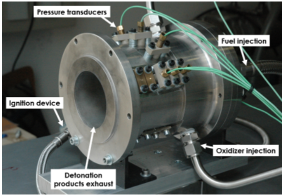
Outline

Non-ideal detonation propagation

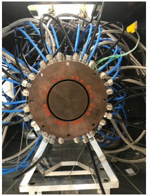
Transportation - detonation in propulsion (1/2)

Rotating Detonation Engines Research at *l'Institut Pprime*[5]

Canteins (2006)



Hansmetzger (2018)



Zitoun (2019)

Working on detonative propulsion since 1996 (PDE and RDE)

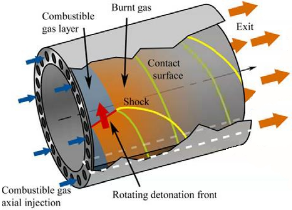
(mostly on applied studies of feasability)

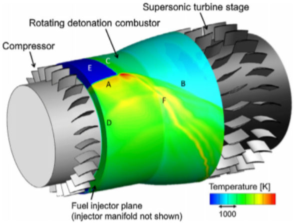
[5] Detonation team works mostly on fundamental (exp., num., theor.) studies on detonation and deflagration dynamics, and $\uparrow p$ / $\uparrow T$ constitutive relations

Transportation - detonation in propulsion (2/2)

Rotating Detonation Engines (RDE)

- Injection at the bottom-end
- Detonation propagation along the circumference
- Burned gases at $\uparrow p \rightarrow$ thrust





Transportation - detonation in propulsion (2/2)

Rotating Detonation Engines (RDE)

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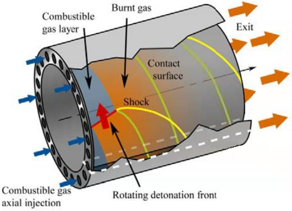
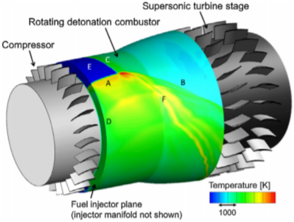
Key issue - highly non-ideal flow with

- Mixing with fuel/burned gases
- 3-D effects
- Discrete injection at high pressure
- **Confinement by burned/inert gases**
- **Chamber curvature**
- **Propagation in narrow spaces**





Overarching goal

Fundamental understanding of non-ideal detonation propagation

How?

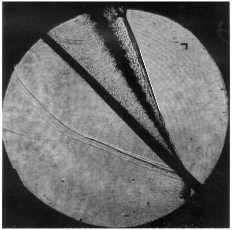
- Through careful experimental and numerical efforts
- Analysis of canonical configurations, i.e., isolating individual effects

Questions

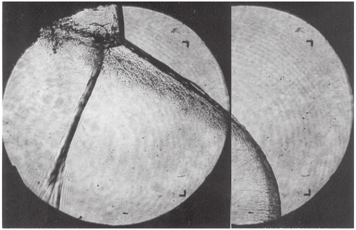
- Can we predict experimental quenching limits?
- Can we reproduce the experimentally observed transmission and propagation dynamics?

Background - sharp vs. diffuse interfaces

Flow fields upon interaction - schlieren images[6]



Sharp interface
$\lambda \gg \delta$



Diffuse interface
$\lambda \ll \delta$ or $\lambda \sim \delta$

[6] Lieberman, D. (2006). Detonation interaction with sharp and diffuse interfaces. *Doctoral Dissertation*. California Institute of Technology.

Background - sharp vs. diffuse interfaces

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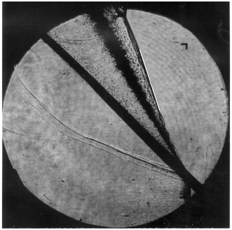

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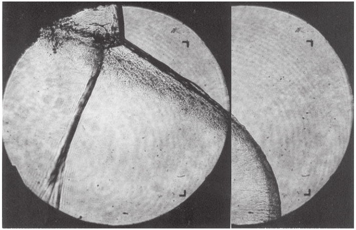


Diffuse interface
$\lambda \ll \delta$ or $\lambda \sim \delta$

Diffuse interfaces more likely upon accidental fuel leaks!

[6] Lieberman, D. (2006). Detonation interaction with sharp and diffuse interfaces. *Doctoral Dissertation*. California Institute of Technology.

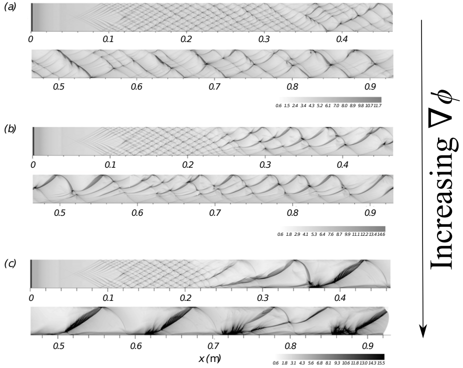
Background - challenges

with using λ to characterize behavior

- Difficult to measure experimentally within layers/interfaces
- λ not uniquely defined even in the absence of gradients
- Properly capturing λ variation in the interface, δ?
- Need to resolve the detonation front!

with inviscid models

- Lack of energy dissipation mechanisms/diffusive processes
- Not adequate for highly unstable mixtures (i.e. moderate to high E_a)
- Solutions do not converge with resolution



Han, W. et al. (2019). JFM, 865, 602-649.

Detonation-diffuse interface interaction

$\Delta\lambda_{\text{crit}}$ for quenching [7]

[7] **Melguizo-Gavilanes, J.**, Peswani, M., & Maxwell, B. M. (2021). Detonation-diffuse interface interactions: failure, re-initiation and propagation limits. Proceedings of the Combustion Institute, 38(3), 3717-3724.

Goal of the study

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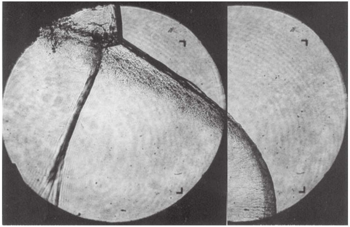
To examine failure/re-initiation mechanisms for detonation-diffuse interface[8] interactions, and determine critical cell size gradients, $\nabla\lambda_{\text{crit}}$, for quenching

Experiment (Lieberman, 2006):



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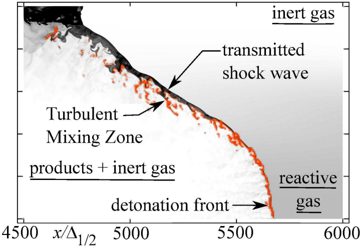

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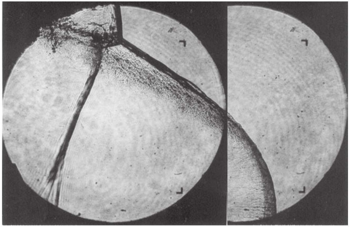

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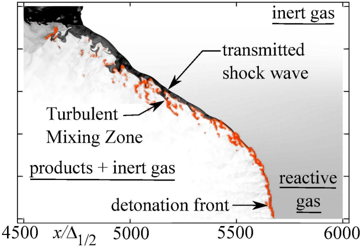


How?

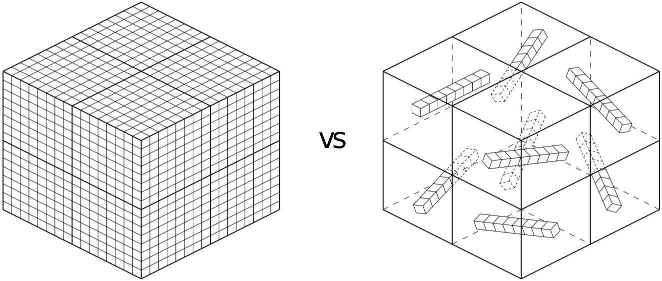
- Numerical simulations using the CLEM-LES methodology

[8]Interface, δ, is **diffuse** if $\lambda \ll \delta$ or $\lambda \sim \delta$

Physical model - proposed methodology

Compressible Linear Eddy Model (CLEM)

- Grid within a grid approach based on the Linear Eddy Model (LEM)[9] - reformulated for compressible flows
- Reduce small scales to 1-D diffusion/reaction problem
- Validated for premixed detonations in channels[10] and DDT[11]



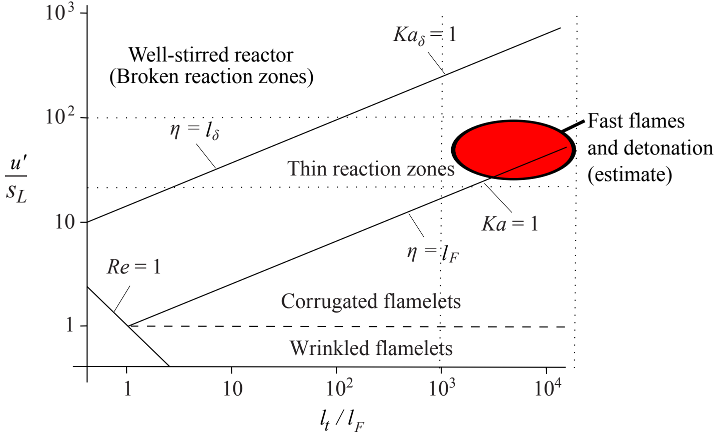
[9] S. Menon and A. R. Kerstein (2011) Turbulent Combustion Modeling: Advances, New Trends and Perspectives, Springer, 2011, Ch. 10: The Linear-Eddy Model, pp. 221-247.

[10] Maxwell, B. et al. (2017). JFM, 818, 646-696.

[11] Maxwell, B. et al (2018). CNF, 192, 340-357.

Physical model - detonation combustion regimes

Borghi-Peters diagram



$$\frac{u'}{s_L} = \frac{\text{turbulence intensity}}{\text{laminar burning velocity}}$$
$$\frac{l_t}{l_F} = \frac{\text{turbulence macroscale}}{\text{reaction zone thickness}}$$

Physical model - LES formulation

On the large scales

$$\frac{\partial\bar{\rho}}{\partial t} + \boldsymbol{\nabla}\cdot(\bar{\rho}\tilde{\boldsymbol{u}}) = 0 \quad \text{(Mass)}$$

$$\frac{\partial(\bar{\rho}\tilde{\boldsymbol{u}})}{\partial t} + \boldsymbol{\nabla}\cdot(\bar{\rho}\tilde{\boldsymbol{u}}\otimes\tilde{\boldsymbol{u}}) + \nabla\bar{p} - \boldsymbol{\nabla}\cdot\bar{\rho}(\nu+\nu_t)\underline{\boldsymbol{S}} = 0 \quad \text{(Momentum)}$$

$$\frac{\partial(\bar{\rho}\tilde{e})}{\partial t} + \boldsymbol{\nabla}\cdot\left((\bar{\rho}\tilde{e}+\bar{p})\tilde{\boldsymbol{u}} - \tilde{\boldsymbol{u}}\cdot\underline{\bar{\boldsymbol{\tau}}}\right) - \left(\frac{\gamma}{\gamma-1}\right)\boldsymbol{\nabla}\cdot\left(\bar{\rho}\left(\frac{\nu}{P_r}+\frac{\nu_t}{P_{r,t}}\right)\nabla\tilde{T}\right) = -Q\bar{\dot{\omega}} \quad \text{(Energy)}$$

with

$$\tilde{e} = \frac{\bar{p}}{\bar{\rho}(\gamma-1)} + \frac{1}{2}(\tilde{\boldsymbol{u}}\cdot\tilde{\boldsymbol{u}}) + k^{sgs} \quad \text{and} \quad \bar{p} = \bar{\rho}\tilde{T}$$

Momentum closure

$$\frac{\partial(\bar{\rho}k^{sgs})}{\partial t} + \boldsymbol{\nabla}\cdot(\bar{\rho}\tilde{\boldsymbol{u}}k^{sgs}) - \boldsymbol{\nabla}\cdot\left(\frac{\bar{\rho}\nu_t}{P_{r,t}}\nabla k^{sgs}\right) = \underbrace{\bar{\rho}\nu_t\underline{\boldsymbol{S}}\cdot(\nabla\tilde{\boldsymbol{u}})}_{\text{production rate}} - \underbrace{\bar{\rho}\epsilon}_{\text{dissipation rate}} \quad \text{(subgrid KE)}$$

where

$$\nu_t = \frac{1}{\pi}\left(\frac{2}{3C_\kappa}\right)^{3/2}\sqrt{k^{sgs}}\bar{\Delta} \quad \text{and} \quad \epsilon = \pi\left(\frac{2}{3C_\kappa}\right)^{3/2}(k^{sgs})^{3/2}/\bar{\Delta}$$

Physical model - CLEM formulation

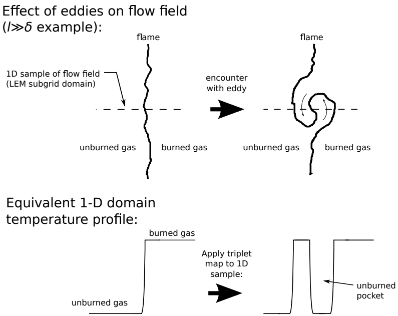
Reaction rate closure on the small scales

$$\rho \frac{DT}{Dt} = \left(\frac{\gamma - 1}{\gamma}\right)\dot{p} + \rho \frac{\partial}{\partial m}\left(\rho\alpha \frac{\partial T}{\partial m}\right) - \left(\frac{\gamma - 1}{\gamma}\right)Q\dot{\omega} + \dot{F_T} \text{ (Enthalpy)}$$

$$\rho \frac{DY}{Dt} = \rho \frac{\partial}{\partial m}\left(\rho \frac{\alpha}{Le} \frac{\partial Y}{\partial m}\right) + \dot{\omega} + \dot{F_Y} \text{ (Reactant mass fraction)}$$

$$\text{where} \quad \dot{\omega} = -\rho A Y \exp\left(E_a/T\right);\; m(x,t) = \int_{x_o}^{x} \rho(x,t)dx; \quad D_T = f(k^{sgs}) = f(C_\kappa)$$

Turbulent stirring



Challenges and physical model recap

Challenges

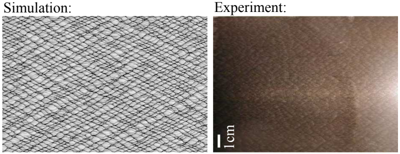
- Interest in industrially relevant scales
- λ not uniquely defined even in absence of reactivity gradients!

Physical model

- LES-filtered Navier-Stokes for a reactive, calorically perfect gas
- 1-step Arrhenius kinetics (closure of $\overline{\dot{\omega}}$ through CLEM subgrid modeling)

Model calibration

- $2.5C_2H_4 + 3O_2$ at $p_0 = 11$ kPa and $T_0 = 300$ K (moderately unstable)[12]
- Kinetic and transport parameters fitted at vN-state (i.e., τ_{ind}, $\Delta_{1/2}$); s_L at postshock state for $M_s = 0.5 M_{\text{CJ}}$
- ν_t and ϵ are $f(C_k, \bar{\Delta}, k^{sgs})$; ($C_k$ and $\bar{\Delta}$ calibrated to reproduce λ_{exp}[13])

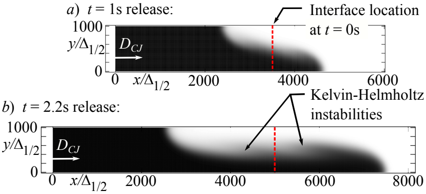


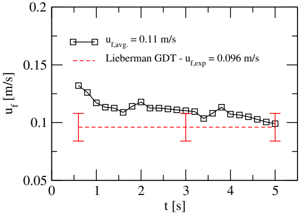
[12] $E_a/R_uT_{\text{vN}} = 28$; $Q/R_uT_{\text{vN}} = 116$; $\gamma = 1.33$
[13] $\lambda_{\text{exp}} \sim 2$ mm

Domain, initial and boundary conditions

2D simulations carried out in two steps

- **Step 1** : Compute gravity current for a $2.5C_2H_4 + 3O_2$ / N_2 interface $p_0 = 11$ kPa and $T_0 = 300$ K; $L_x \sim 1.0 \times L_y \sim 0.15$ m (5 s/1 m) - OpenFOAM
- **Step 2** : Take fields as initial condition, map N_2 field to mass fraction $Y = 1 - Y_{N_2}$; $L_x \sim 0.8 \times L_y \sim 0.1$ m - non-ideal detonation/CLEM-LES[14]



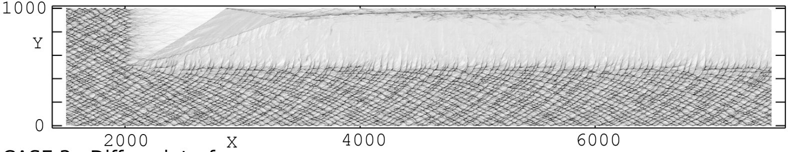


[14]**Resolution**: $\bar{\Delta}_{\text{LES}} = \Delta_{1/2}/8$, $N = 16$ subgrid elements per cell ($\bar{\Delta}_{\text{eff}} = \Delta_{1/2}/128$) (Scale: 1 cm $= 100\Delta_{1/2}$)

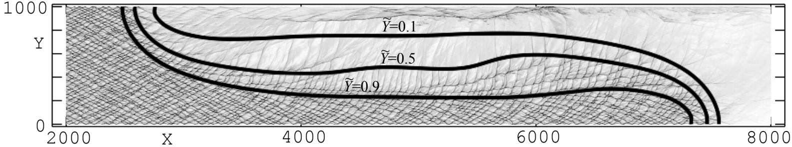
Results - overall dynamics

Soot foils

CASE 2: Sharp interface (0°)



CASE 3: Diffuse interface



Results - overall dynamics

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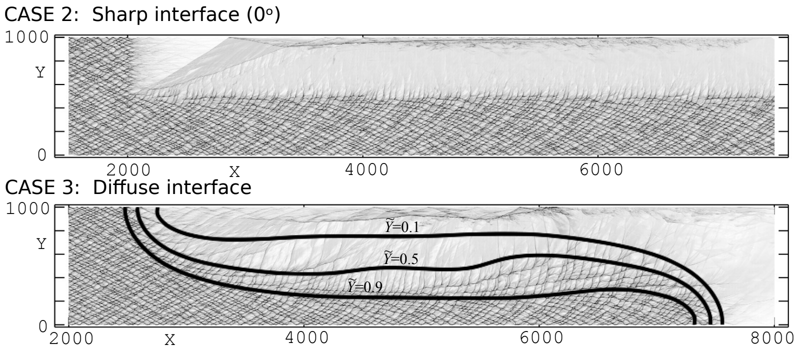
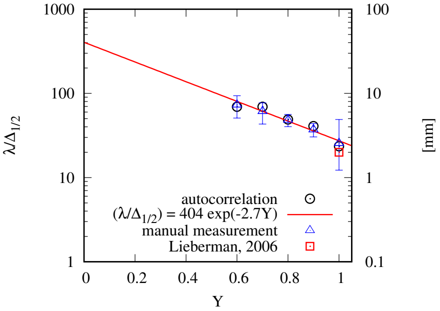


Diffuse interface case exhibits quenching and re-initiation in δ!

Results - overall dynamics

Mapping Y to λ to capture proper cell size dynamics[15]



[15] Required separate premixed detonation simulations

Results - overall dynamics

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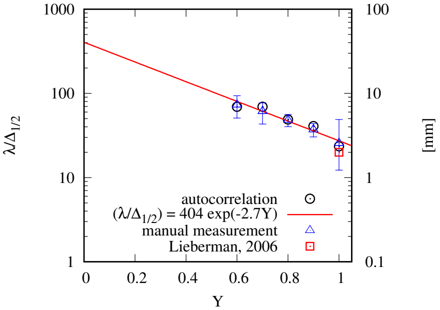
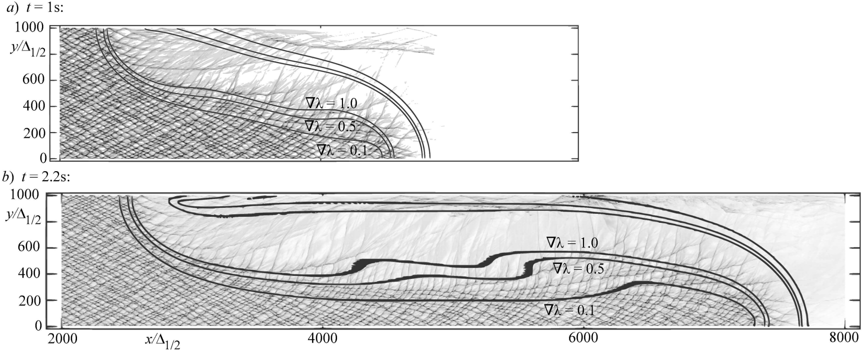


Cell size gradient can be computed via $\nabla\lambda = (d\lambda/dY)\nabla Y$

[15] Required separate premixed detonation simulations

Results - overall dynamics

Cell size gradient superimposed on soot foils



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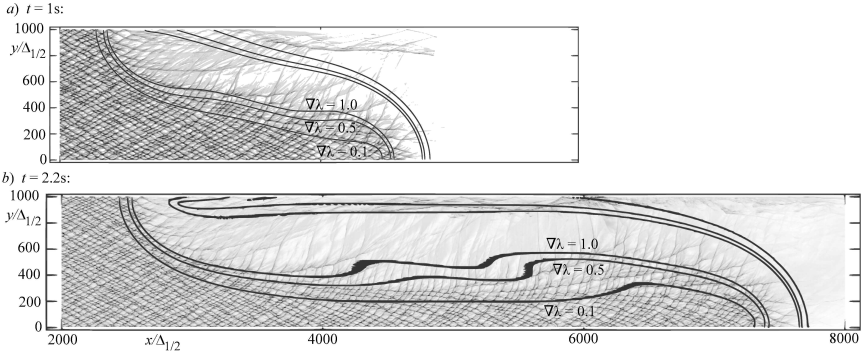
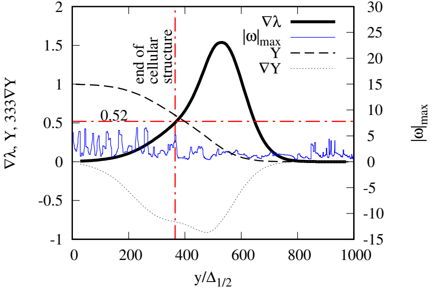


$\overline{\nabla\lambda_{\mathbf{crit}}} \sim 0.5 \rightarrow$ **direct consequence of cellular dynamics within the interface**

Results - critical conditions

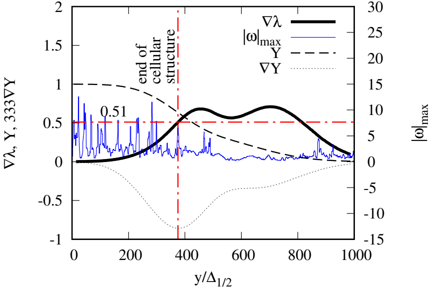
Determination of $\nabla\lambda_{crit}$

Gravity current at $t = 1.0$ s



$x = 4000\Delta_{1/2}$ (40 cm)

Gravity current at $t = 2.2$ s



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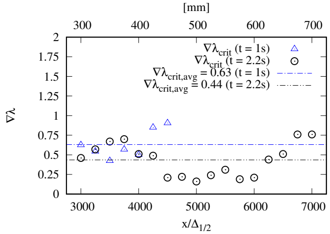
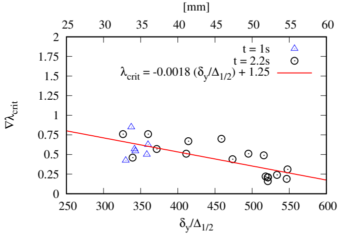
Results - $\nabla\lambda_{crit}$, quenching and re-initiation

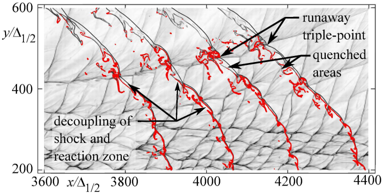
Critical detonation cell size gradient

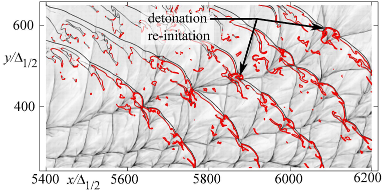




↑ δ favors detonation transmission

Quenching, re-initiation within δ





Triple point transmission characteristic of deto-diffuse interface interactions

Discussion and closing remarks

Applicability of reported $\nabla\lambda_{\mathbf{crit}}$

- In agreement with previous work - $\uparrow \delta$ favors detonation transmission

[16] Kryuchkov, S. I. et al. (1996). PROCI (Vol. 26, No. 2, pp. 2965-2972); Kuznetsov, M. S. et al. (1998). PROCI (Vol. 27, No. 2, pp. 2241-2247)

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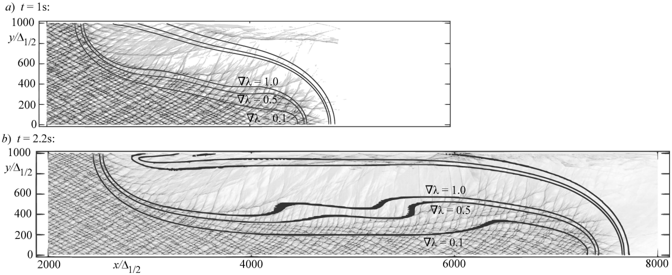
Deto-diffuse interface interaction - main take away[17]

Detailed investigation of $\nabla\lambda_{\text{crit}}$ for quenching at industrially relevant scales using CLEM-LES

Soot foils for detonation-diffuse interface interaction



Key result: $\overline{\nabla\lambda_{\text{crit}}} \sim 0.5 > 0.1$ (value reported in literature) $\rightarrow$ direct consequence of cellular dynamics within the interface

[17] **Melguizo-Gavilanes, J.**, Peswani, M., & Maxwell, B. M. (2021). Detonation-diffuse interface interactions: failure, re-initiation and propagation limits. Proceedings of the Combustion Institute, 38(3), 3717-3724.

Acknowledgments

HPC resources provided by the Core Facility for Advanced Research Computing at CWRU

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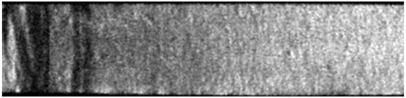

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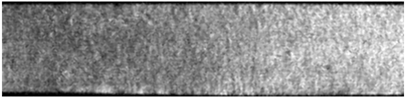

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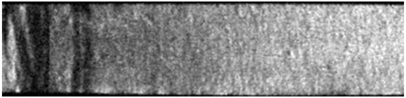

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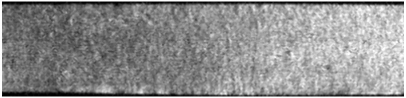

Special thanks to

Prof. Dirk Roekaerts and the Dutch Section of the Combustion Institute