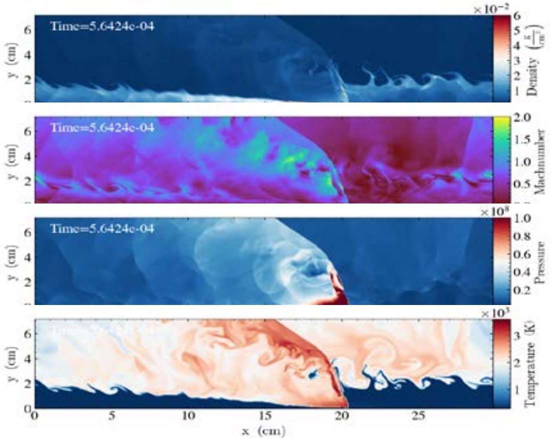
COMPUTATIONAL STUDY OF VARIABLE FUEL-AIR RATIO AND HYDROGEN DOPING IN A ROTATING DETONATION ENGINE



2D RDE simulation results obtained using PeleC

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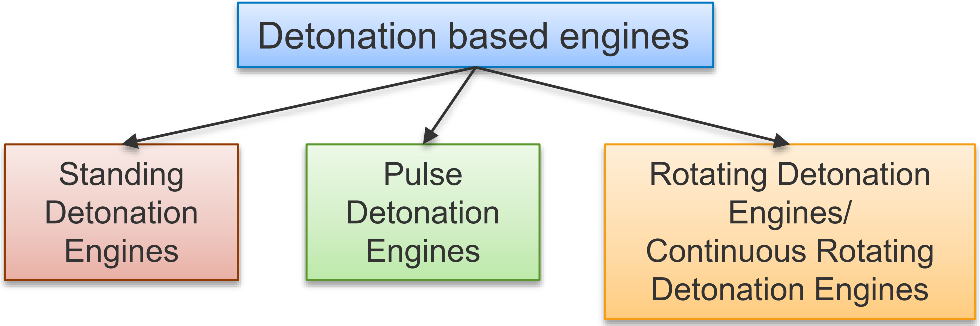
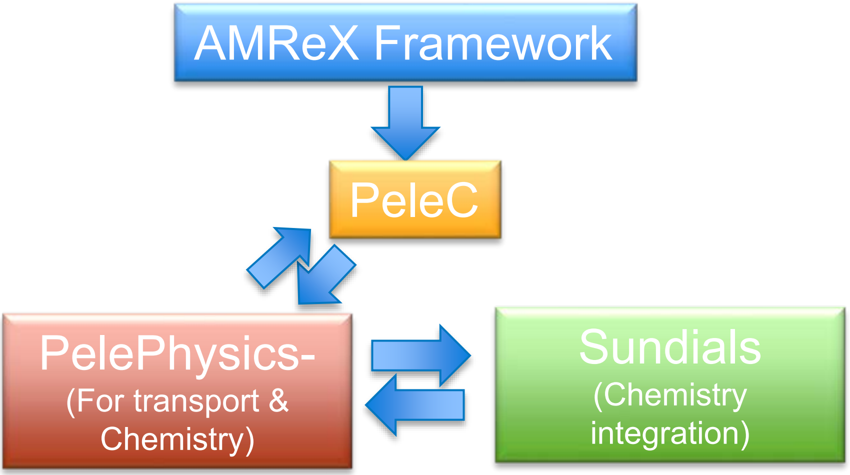
Introduction and objectives



Objective: Study effect of fuel composition on RDE performance using

- Simplified, periodic 2-D geometry
- Automatic mesh refinement (AMR) + High accurate numerical schemes
- Detailed chemistry+ Realistic Transport

PeleC- solver structure



Governing Equations

$$\frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho \mathbf{u}) = 0,$$

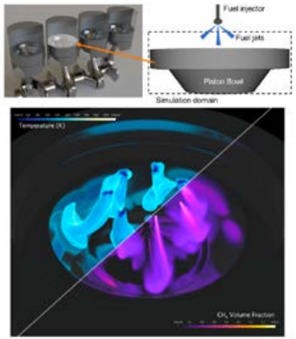
$$\frac{\partial}{\partial t}(\rho Y_k) + \nabla \cdot (\rho \mathbf{u} Y_k) = -\nabla \cdot \boldsymbol{\mathcal{F}}_k + \rho \dot{\omega}_k,$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \nabla \cdot \boldsymbol{\Pi},$$

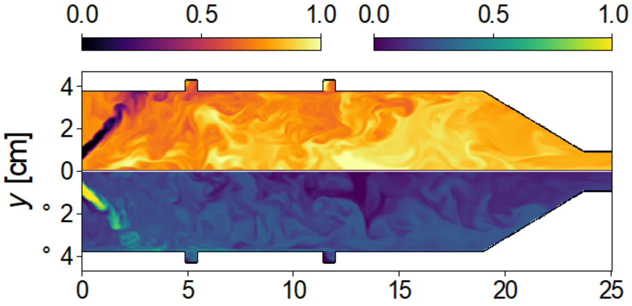
$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho \mathbf{u} E + p\mathbf{u}) = \nabla \cdot \boldsymbol{\mathcal{Q}}.$$

Equations of state: Ideal gas, Suave Redlich-Kwong model
Transport Model: Mixture averaged transport
Second order FVM in space (Piecewise periodic method , Method of Lines) and time (Runge-Kutta 2-step method)

Direct fuel injection in supersonic cavity flame-holder[1].



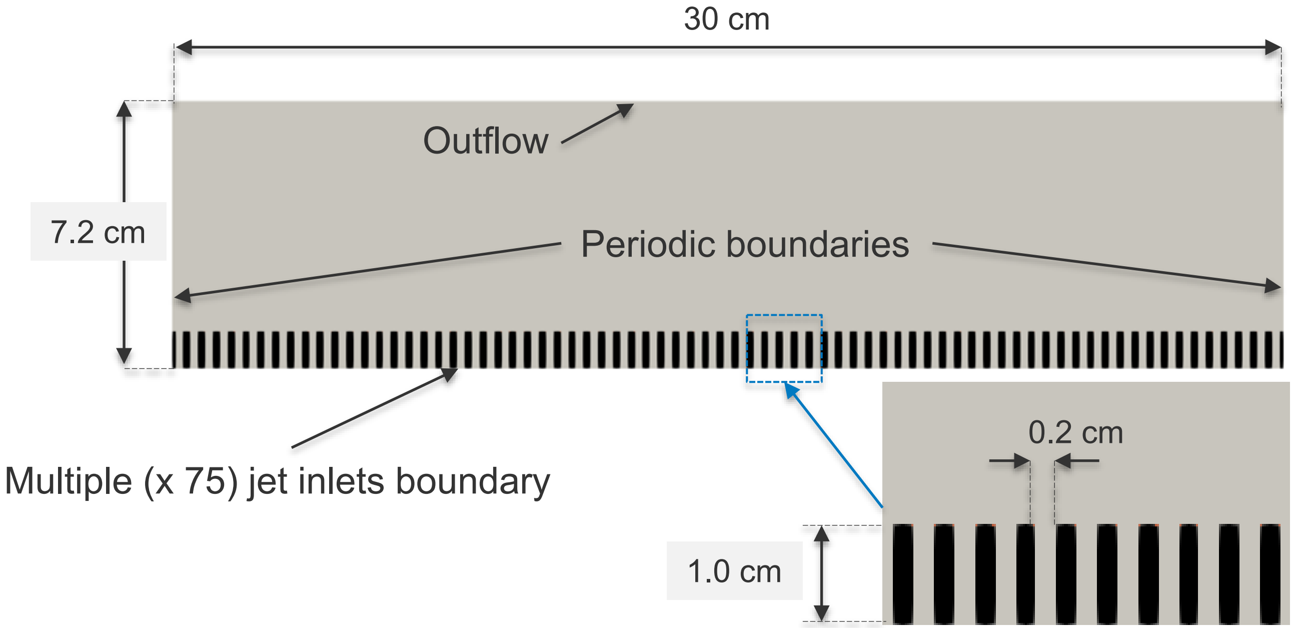
Piston Bowl geometry



Supercritical CO2 power cycle[2]

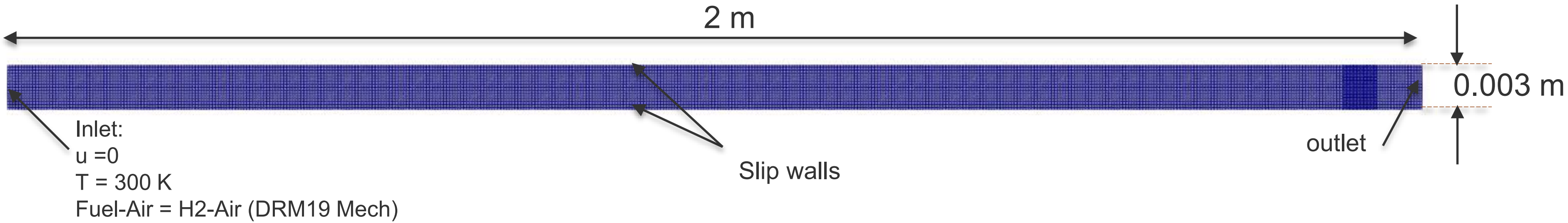
Computational Domain and Boundary Conditions

3D Cylindrical geometry “unrolled” to form 2D, periodic geometry



Mesh sensitivity study using 1D detonation wave

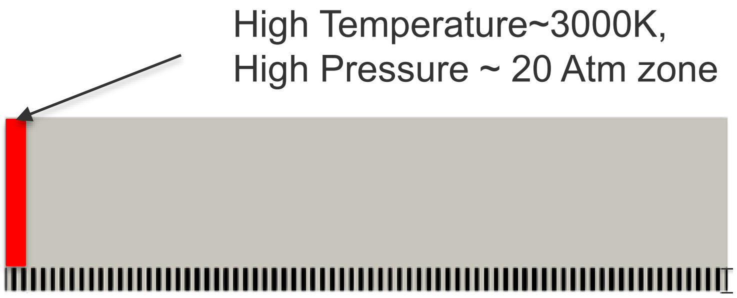
Computational domain (not to scale) and boundary conditions



	Grid 1	Grid 2	Grid 3
No of AMR levels	0 (uniform single grid)	1	2
Refinement ratio(RR)	2	2	2
Δx_{min} (micrometers)	384	192	96
Computed Detonation Speed (m/s)/ CJ-Speed (m/s)	1970/1976	1973/1976	1974/1976

Grid 2 with 2 levels and RR of 2 selected for study

Simulation Setup



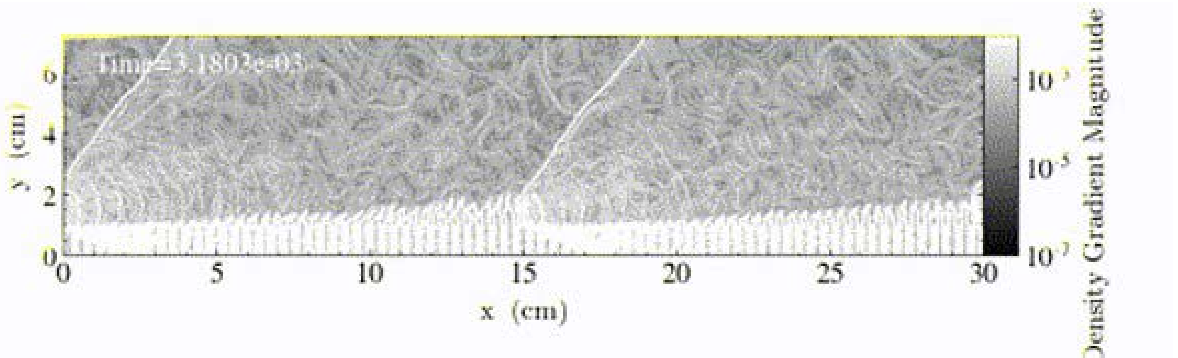
Boundary condition implementation (P= interior pressure):
If $P>P_0$ → Treat inlet as wall
$P_0>P>P_{cr}$ → Gas dynamics based relations for T, V
$P<P_{cr}$ → Chocked flow relations

Numerical Scheme: MoL with Godunov Scheme
Time Integration: Second-order Runge Kutta
Max. AMR Level: 2
Chemistry: DRM19 / LeDryer
Transport: Ideal gas

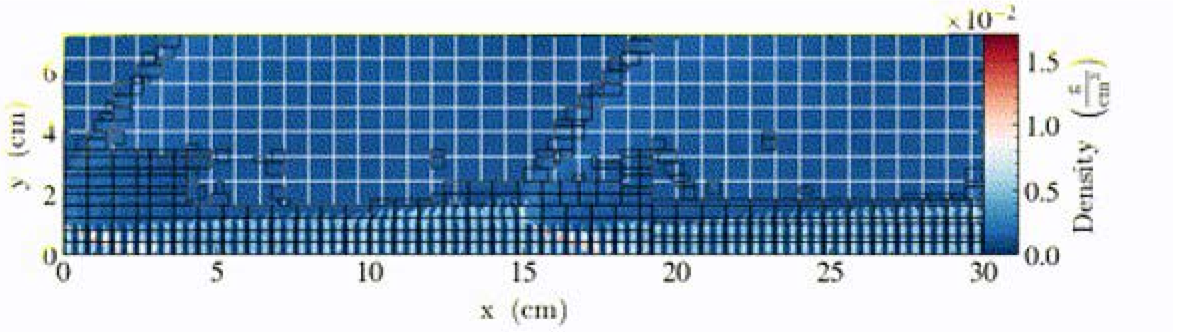
Simulations (P_0=10 Atm, T_0=500K)	Fuel Composition (mole fraction)
Case 1	H2: 1.0, CH4: 0.0
Case 2	H2: 0.9, CH4: 0.1
Case 3	H2: 0.8, CH4: 0.2
Case 4	H2: 0.5, CH4: 0.5

Automatic mesh refinement using PeleC (Case:3)

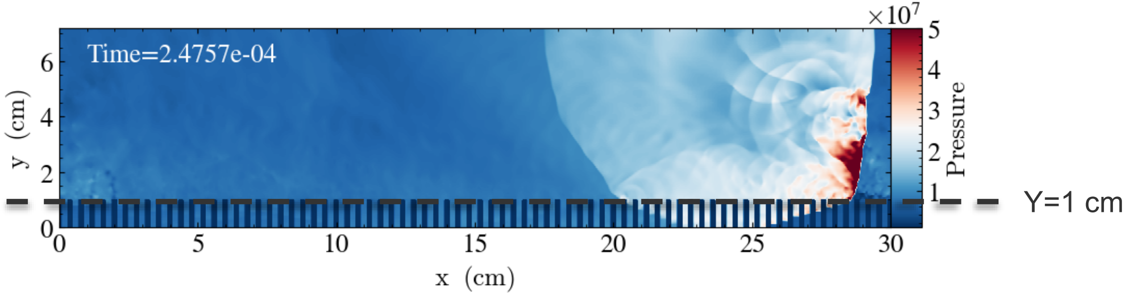
Numerical schlieren

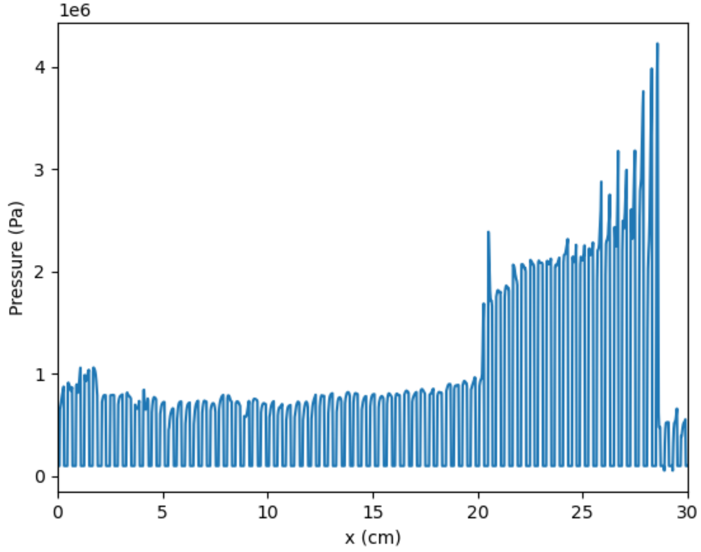


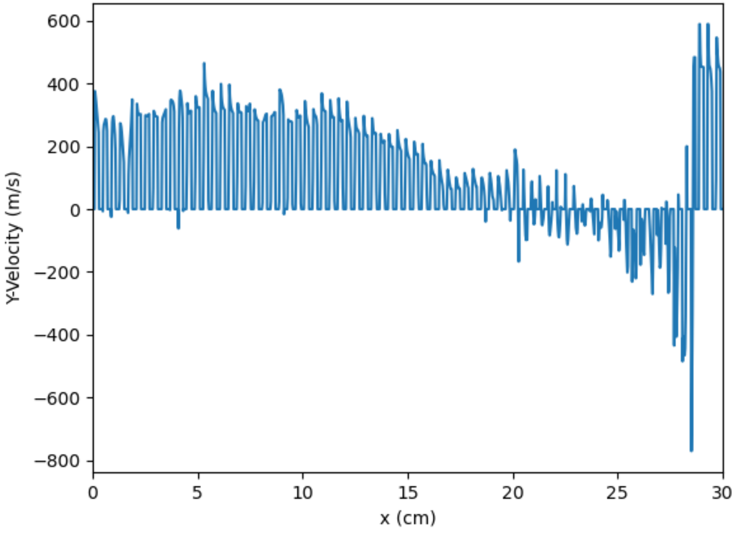
AMR boxes generated during simulation



Instantaneous fuel injection and pressure profile





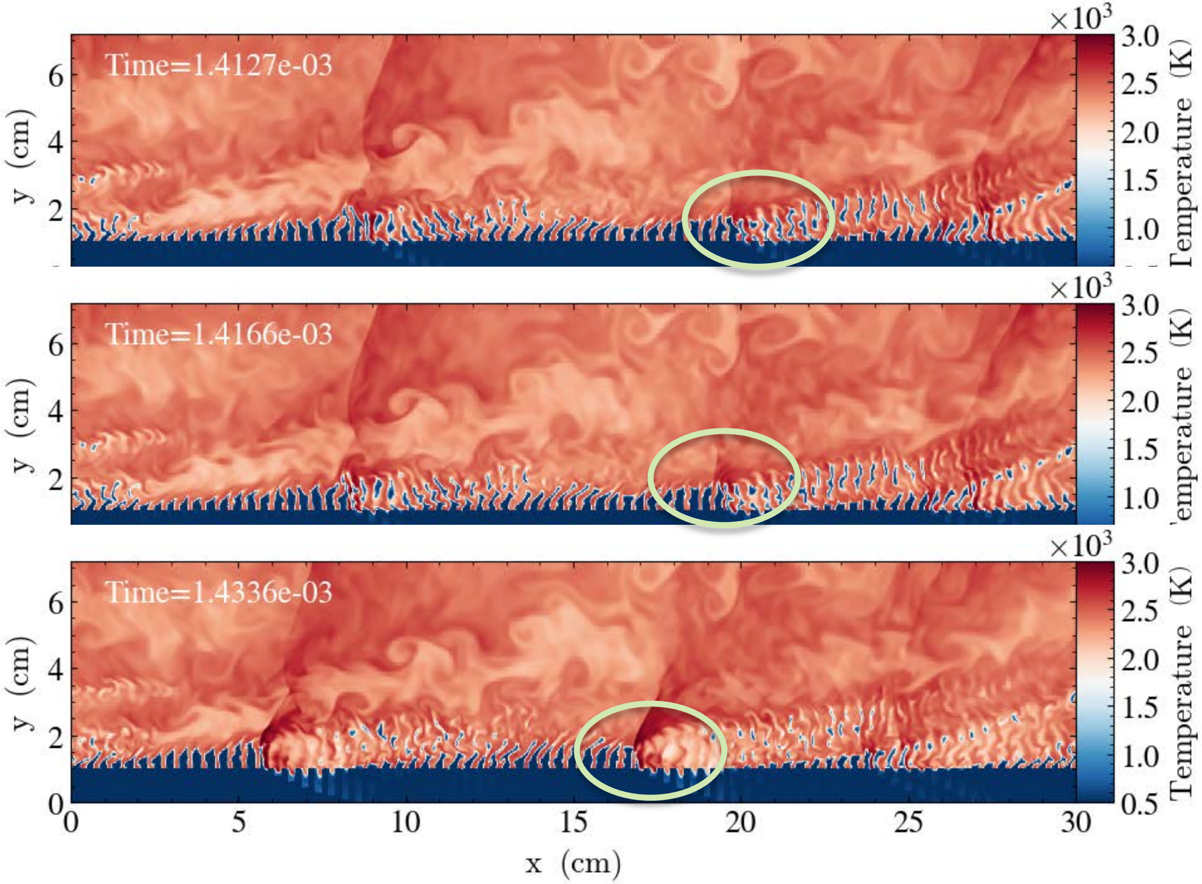


Sequence leading to micro-detonations

Fuel-air+product mix

Deflagration

Transition to detona

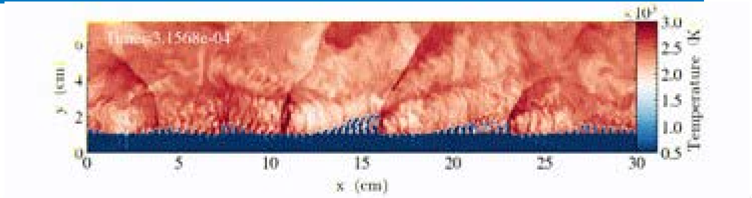


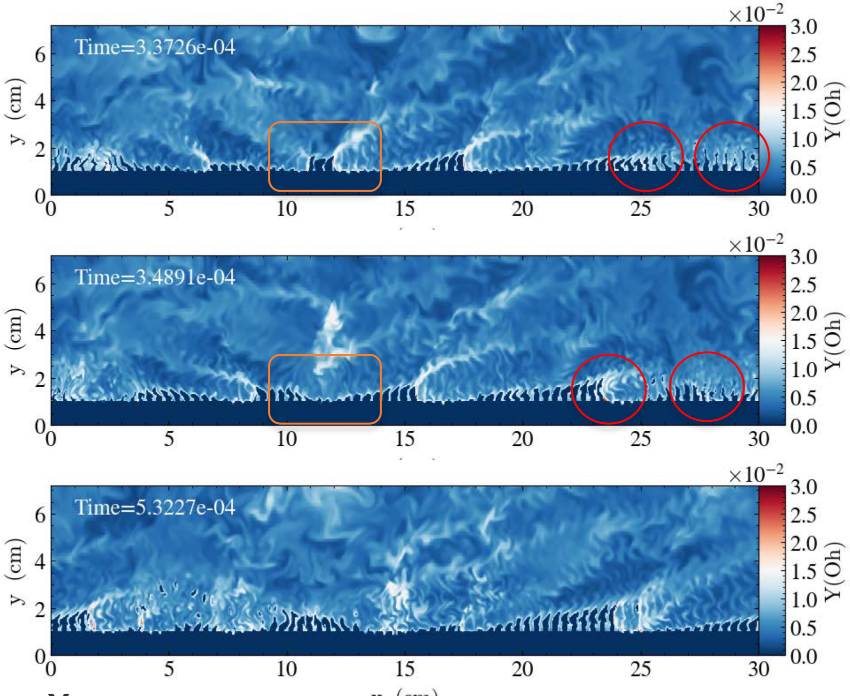
Ignition and transients before stable waves formation (Case 1: $H2=100\%$)

fuel-air -products → Quicker autoiginition → Micro-detonations

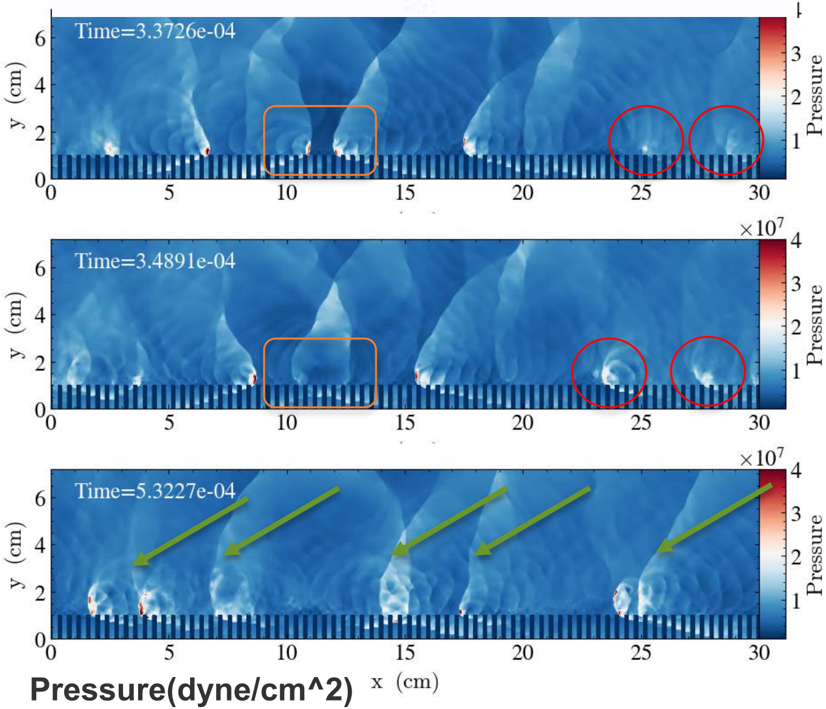
Counter moving wave collision → Reduction of strength

Unidirectional waveset generation





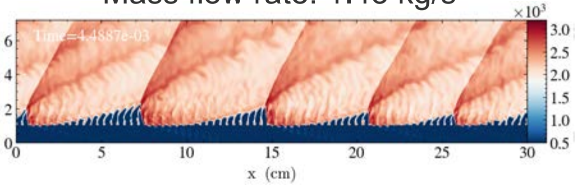
Y_{OH}



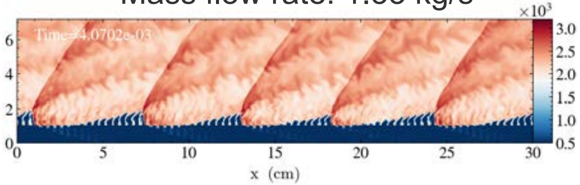
Pressure(dyne/cm^2)

Flow structures and waves

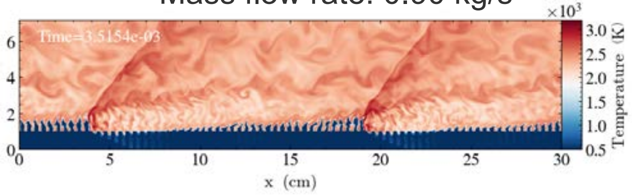
Case 1: (H2:100%)
# of waves=5
T= 4.5 ms
Mass flow rate: 1.43 kg/s

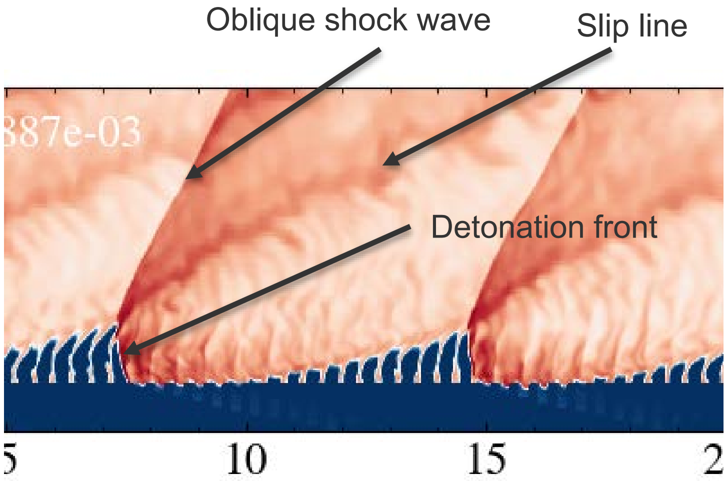


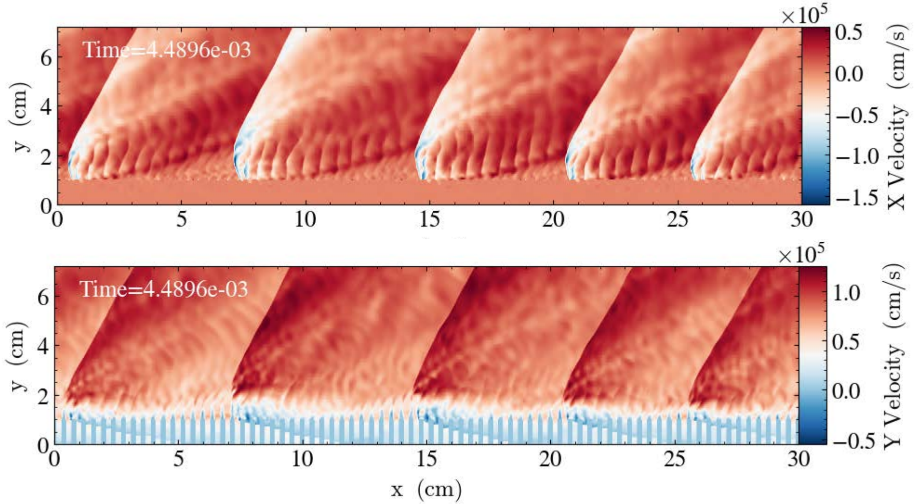
Case 2: (H2:90%)
# of waves=5
T= 4 ms
Mass flow rate: 1.33 kg/s



Case 3: (H2:80%)
# of waves=2
T = 3.5 ms
Mass flow rate: 0.90 kg/s



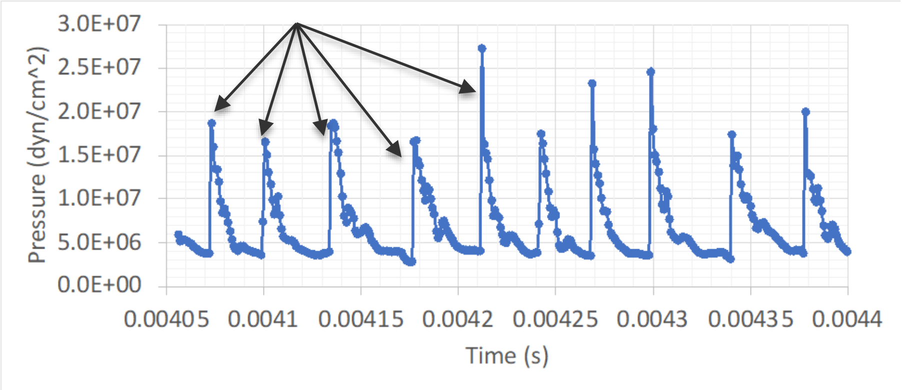




X- and Y- velocities, time=4.5 ms, CASE1

Detonation wave speeds and frequencies

5 detonation waves



Pressure time series, CASE 1

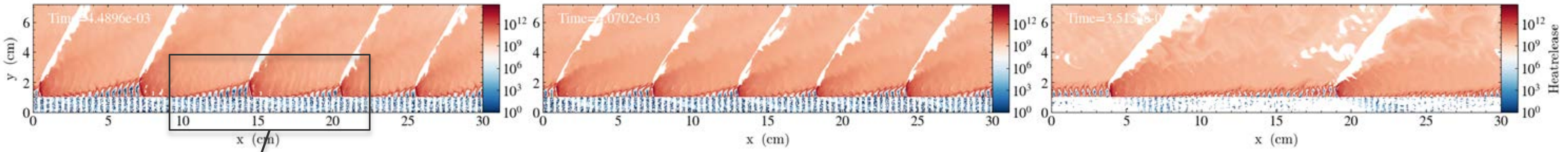
	Case 1	Case 2	Case 3
Frequency (kHz)	5.94	5.76	5.60
Detonation speed (m/s)	1781.8	1728.4	1674.4
CJ-Speed (m/s)	1952	1904	1874

Reactions and detonation ratio

Case 1: (H2:100%)
# of waves=5

Case 2: (H2:90%)
# of waves=5

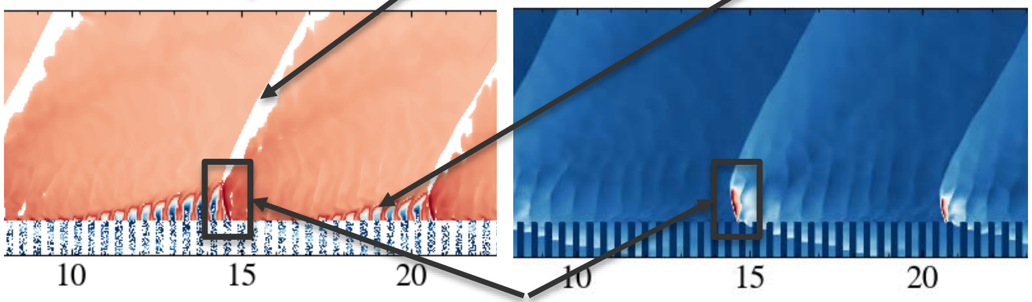
Case 3: (H2:80%)
# of waves=2



$$\eta_{Det-Def.ratio} = \frac{Heat\ release\ due\ to\ detonation}{Total\ Heat\ Release}$$

Negative HR zones

Deflagration zones



Heat release rate

Detonation zone

Pressure

	Case 1	Case 2	Case 3
$\eta_{Det-Def.ratio}$	72.3%	71.2%	58.85%

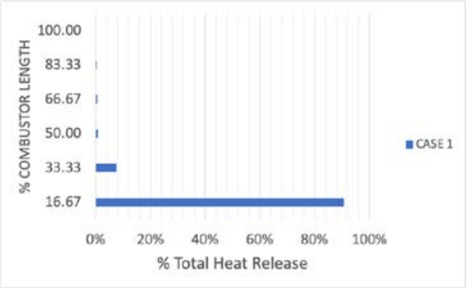
Axial heat release and dynamic pressure distribution

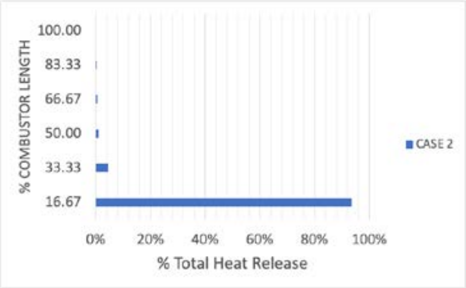
CASE 1

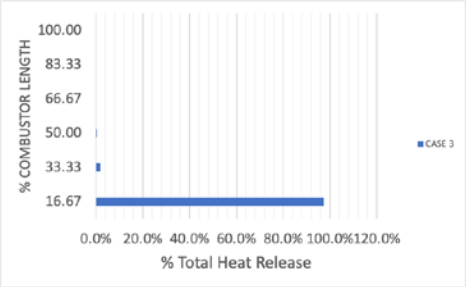
CASE 2

CASE 3

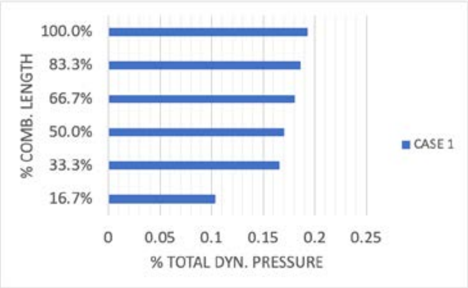
Heat Release Distribution

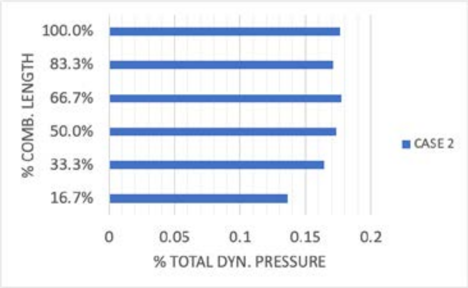


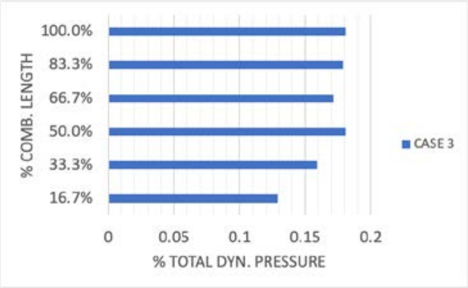




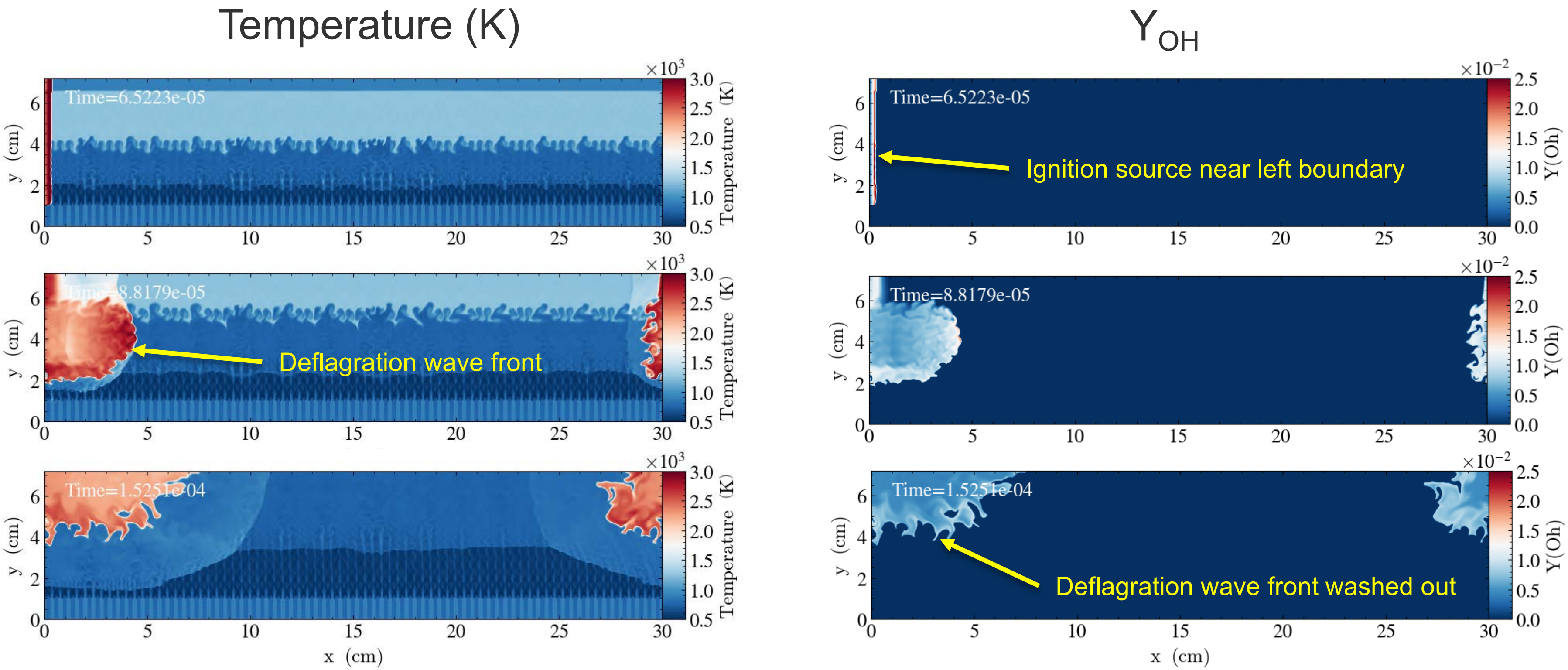
Dynamic Pressure Distribution







Ignition and transients: unsustainable waves (Case 4: H_2=50%)



Conclusions

- AMR based compressible, reactive solver used to simulate 2D flow in a simplified RDE geometry
- Initial transients of RDEs showed multiple and micro detonations, constantly interacting, colliding, coalescing and dissipating but finally forming unidirectional waves
- Effect of CH_4 addition changes reactivity: Stable detonation fronts not found for CH_4 composition >20%
- For specified P_0, T_0, CH_4:20% case showed 2 detonation fronts while lower CH_4 composition showed 5 waves
- The calculated detonation speeds decreased with increasing CH_4 concentration and matched well with C-J speeds
- Combustion efficiency also reduced for CH_4 concentration of 20% due to more burning occurring from deflagration

References

1. Adaptive mesh based combustion simulations of direct fuel injection effects in a supersonic cavity flame-holder, Hariswaran et.al., Combustion and Flame, Vol. 232, 2021
2. High-fidelity numerical simulation study of oxy-combustor: Impact of equation of state model, M.T.H. de Frahan et. al., 18th International Conference on Numerical Combustion, San Diego, 2022

Thank You

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