Numerical Study on the Effect of Methane Doping in Hydrogen-Air Rotating Detonation Engines for various Temperatures and Pressures

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Rotating Detonation Engines

- Gas turbine (GT) engines are the most popular devices today for transportation and power generation purposes. However, scientific community looks forward to new technologies that produce energy even more efficiently. In contrast to the Brayton cycle on which GT engines work, detonation cycle operates at constant volume and a static pressure gain. Hence, it produces more work output when compared to the Brayton cycle (Figure 1).

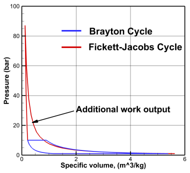

Figure 1: *Comparison of Brayton and Detonation cycle*

- Detonation cycle is used in devices such as Standing Detonation Engines (SDEs), Pulse Detonation Engines (PDEs) and Rotating Detonation Engines (RDEs). RDEs have gained more scientific interests recently because,
  - of their lower entropy generation and hence higher efficiency when compared to GT engines
  - detonation needs to be initiated only once
  - faster fuel consumption rate and hence higher power output
  - pressure increase from detonation reduces the load on compressors

Figure 2: *(a) A conceptual rotating detonation turbojet engine [1] (b) The combustion chamber of an Rotating Detonation Engine (RDE) [1]*

- The goal of this work is to perform numerical simulations to study detonation and combustion occuring inside an RDE engine.

PeleC CFD Solver

- PeleC [2] is a CFD solver application funded by the US Exascale Computing Project for simulating compressible reactive flow in complex geometries and using adaptive mesh refinement (AMR). PeleC is based on the AMReX framework [3] which supports Cartesian, block-structured, AMR capabilities on both CPU and GPU architectures.

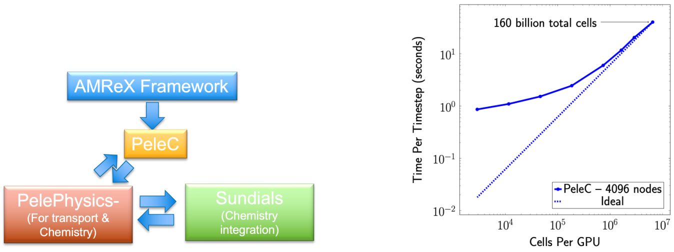

Figure 3: *(a) PeleC application architecture (b) Strong scaling of premixed flame test case computed using 4096 Summit nodes*

- Key features of the PeleC software suite include:
  - Compressible, reactive Navier-Stokes formulation
  - Piecewise Parabolic Method (PPM) and Method of Lines (MOL) space discretizations
  - Second-order accuracy in space and time (Runge-Kutta two-stage (RK2))
  - Supports real gas equation of state
  - Mixture-averaged transport models and
  - Species transport framework including reduced and detailed mechanisms
  - Embedded Boundary (EB) representation for complex geometries

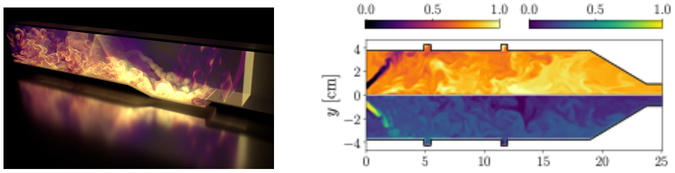

Figure 4: *Applications of PeleC solver. (a) Simulation of direct fuel injection in a supersonic cavity flame holder [4, 5] (b) Simulation of reactive flow inside a supercritical CO2 cycle based combustor*

Numerical Results

Computational domain and boundary conditions

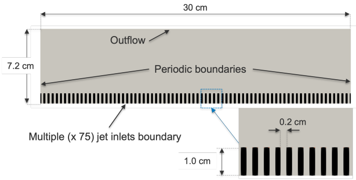

Figure 5: *Computational domain and boundary conditions used in this study*

- 3D annular combustion chamber is 'unwrapped' to obtain a 2D rectangular domain with discrete, premixed, fuel-air jets with specified upstream total pressure and temperature at the inlets.

Effect of AMR

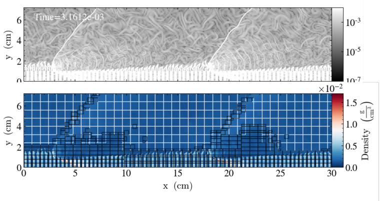

Figure 6: *Numerical Schlieren (top) and the corresponding refinement grid zones (bottom) outlined in black color*

- AMR resolves detonation and shock zones at increased resolutions to capture fine-scale dynamics

Flow field and wave structure

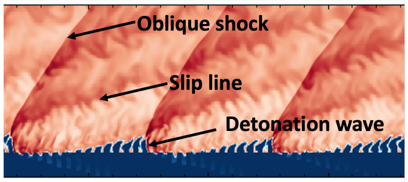

Figure 7: *Stable detonation and flow structure*

- Under stable operating conditions, single or multiple continuously rotating wave structures are obtained. Each wave structure consists of a detonation wave, an oblique shock wave and a slip line.

Reaction zones

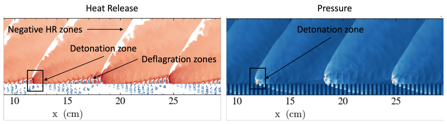

Figure 8: *Detonation and deflagration zones*

- Periodic motion of the detonation front consumes the freshly injected premixed gas. Downstream regions comprise intense mixing of high temperature burnt products and freshly injected fuel-air mixture creating deflagration zones. Negative heat release zones are observed downstream of oblique shocks due to radical species production

Effect of CH_4 doping

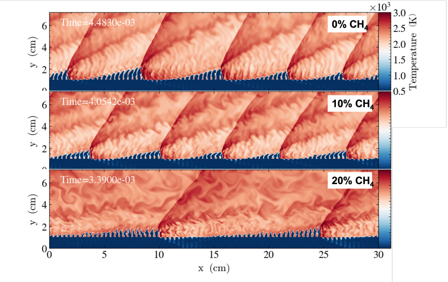

Figure 9: *Effect of CH_4 doping on the number of detonation waves.(T=500K,P=10 Atm)*

- Increasing CH_4 doping reduces fuel-air mixture reactivity. Lower reactivity leads to delayed detonation transition and hence fewer number of detonation wave fronts. Increasing CH_4 doping reduces fuel-air mixture reactivity. Lower reactivity leads to delayed detonation transition and hence fewer number of detonation wave fronts.

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[1] R. Zhou, D. Wu, and J. Wang, "Progress of continuously rotating detonation engines," *Chinese Journal of Aeronautics*, vol. 29, no. 1, pp. 15–29, 2016.

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