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Three-dimensional detonation structures and effects of thermal confinement in a linear channel

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A R T I C L E I N F O

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A B S T R A C T

This study employs three-dimensional (3D) numerical simulations to investigate the detonation wave propagation in an unwrapped annular combustor configuration, focusing on thermal confinement effects on detonation structures and blast dynamics. The compressible Navier-Stokes equations are solved for stoichiometric kerosene-air mixtures under three distinct wall boundary conditions: (1) adiabatic (uncooled), (2) isothermal at 300 K (representing actively cooled walls), and (3) hybrid adiabatic-isothermal configurations. Results reveal that wall temperature critically governs detonation morphology: adiabatic boundaries produce regular cellular structures via 'multi-kernel' formation (intersections of four transverse waves), while cooled walls (300 K) generate stripe-like 'line-kernel' (formed through two-wave intersections), accompanied by double-wave structures, increased pressure fluctuations, and unburned fuel pockets. The hybrid case demonstrates asymmetric detonation development, with stable propagation on the adiabatic side contrasting with elongated cells and intensified wave-wall interactions on the cooled side. Quantitative analysis shows that cooled boundaries reduce the detonation wave height compared to adiabatic cases and promote irregular cell sizes due to suppressed boundary layer reactions. These findings present the first systematic evidence of 3D thermal confinement effects on RDW dynamics, revealing a critical trade-off in combustor design: while lower wall temperatures enhance material durability, they compromise combustion efficiency through increased flow unsteadiness and incomplete fuel consumption. The study advances the fundamental understanding of detonation physics in practical thermal gradients and provides actionable insights for optimizing cooling strategies in rotating detonation engines.

1. Introduction

Detonation waves have been explored extensively for potential utilisation in propulsion systems owing to their advantages over deflagration waves. Amongst proposed detonation-based engines, the rotating detonation engine (RDE) employs a continuously propagating rotating detonation wave (RDW) in an annular combustion chamber (termed the rotating detonation combustor, RDC). Within this confined environment, boundary conditions can significantly influence RDW propagation [1]. For engineering applications, active cooling is frequently implemented to reduce RDC wall temperatures and improve material durability. Hence, understanding the influence of thermal confinement on RDW propagation and structure becomes essential for developing effective cooling strategies to optimise RDE performance.

RDWs exhibit cellular structures resulting from interactions between leading shock waves, transverse shock waves, and Mach stems. Most experimental studies of detonation cellular structures have depended on two-dimensional (2D) representations, where structures are recorded on tube or chamber walls using soot foils or optical diagnostics. There are descriptions of three-dimensional (3D) regular cellular structures in the literature [2–4]. Nevertheless, time-resolved 3D measurements of detonation dynamics under thermal confinement conditions remain scarce, hindering the understanding of 3D detonation structure evolution.

The interactions between detonation structures and thermal boundary conditions are complex and multifaceted. For instance, higher wall temperatures can enhance local reaction rates and hasten wave propagation but might equally intensify thermal stresses upon materials. Existing studies on thermal confinement effects on RDW propagation and structures remain limited [5]. Certain pioneering work has indicated that RDWs propagate faster at higher wall temperatures [6]. Wang et al. [6] used Reynolds-averaged Navier-Stokes (RANS) simulations

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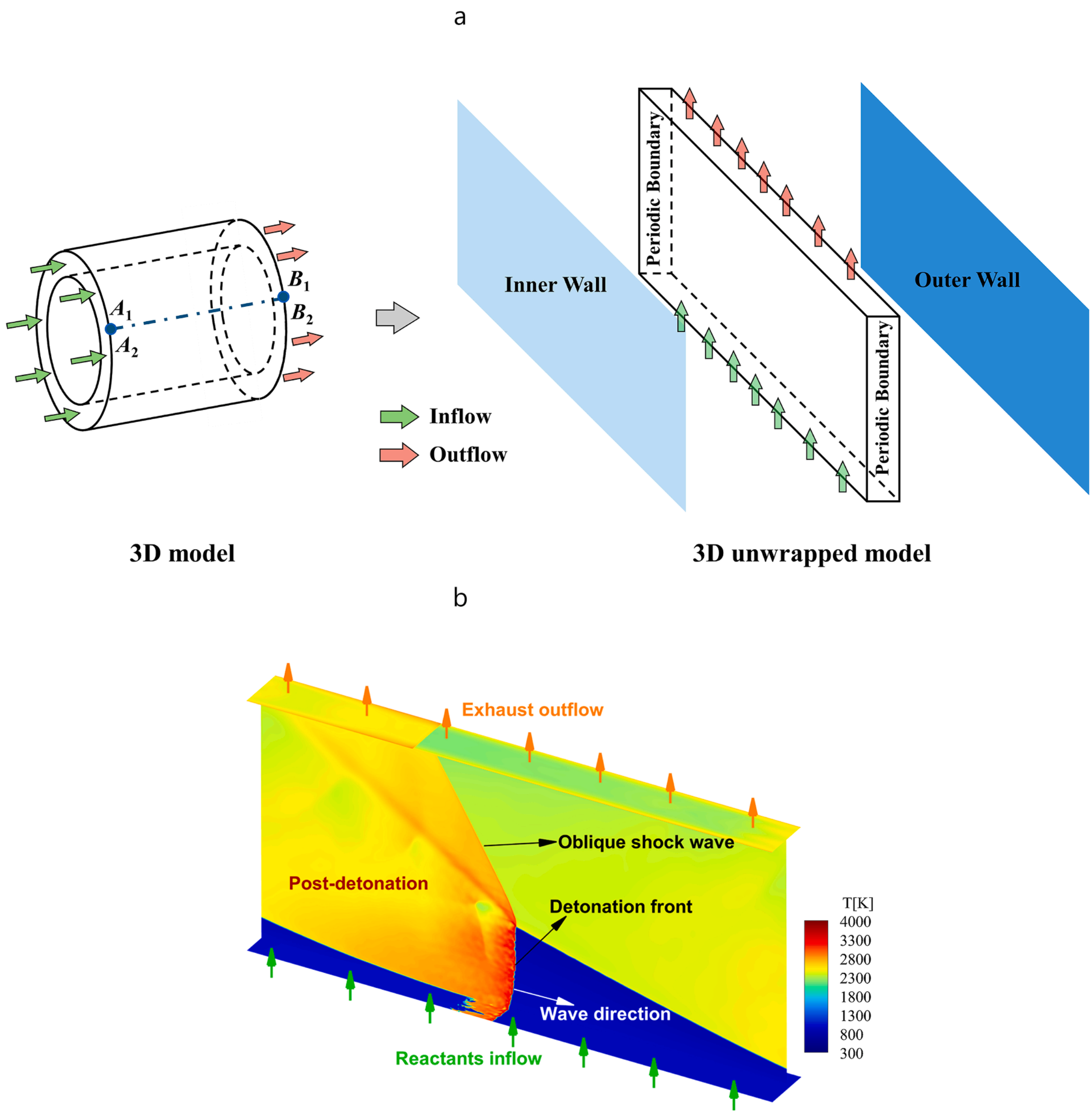

Fig. 1. Schematics of the configuration with boundary conditions (a) and flow structures in the unwrapped RDC model (b).

with a one-step hydrogen-oxygen reaction model to explore thermal wall effects upon RDWs, finding that raised wall temperatures heat boundary regions, thus increasing reaction rates and detonation speeds. Yet, these 2D simulations merely captured side views of RDWs, lacking detailed detonation structures. Wu et al. [5] performed 3D RDC simulations with a one-step chemical model, examining wall temperatures of 300 K, 600 K, and 900 K. Their results revealed detonation quenching at 300 K and 900 K, with stable propagation solely at 600 K. Owing to coarse mesh resolution, their study failed to resolve cellular structures or scrutinise quenching mechanisms. Similar numerical studies by Liu et al. [7] produced no further insights. Together, these works underscore a paucity of understanding of thermal confinement effects upon RDW structures.

This study aims to address this gap by exploring the 3D structural response of RDWs to varying wall thermal conditions through simulations of RDW propagation in a lab-scale RDC fuelled with pre-evaporated kerosene gas [8]. The compressible reactive flows are simulated using high-order numerical schemes alongside a reduced kerosene/air chemical mechanism. Three scenarios have been assessed: adiabatic walls (representing uncooled conditions), isothermal walls at 300 K (emulating active cooling), and a hybrid adiabatic-isothermal configuration (active cooling on one side). These cases represent extremes of thermal boundary conditions, yielding insights into the complete range of RDW behaviours. The present work seeks to clarify the complex dynamics of 3D RDWs and the critical role of wall temperatures in dictating their propagation characteristics.

2. Approach and numerical setup

2.1. Numerical method

The unsteady, compressible, reactive Navier-Stokes equations are solved within a Eulerian framework using a well-established in-house solver [9,10], validated for predicting detonation wave characteristics including propagation speed, pressure profiles, and cellular structure dimensions. The governing conservation equations (mass, momentum, and total energy) are discretised on a uniform Cartesian grid using a finite difference approach, with the following numerical treatments:

- *Convective terms*: Discretised via the weighted essentially non-oscillatory (WENO-LF) scheme with sixth-order spatial accuracy

Table 1
Details of simulated cases.

Case #	Inner Wall	Outer Wall
IaOa	Adiabatic	Adiabatic
ItOt	Isothermal: 300 K	Isothermal: 300 K
IaOt	Adiabatic	Isothermal: 300 K

- *Viscous terms*: Evaluated using a sixth-order central difference scheme

The simulations employ a validated two-step kerosene kinetics mechanism [9]. Transport properties (species viscosity, thermal conductivity, and binary diffusion coefficients) are determined from kinetic theory.

2.2. Physical model and simulation setup

A simplified linear channel configuration that represents an unwrapped annular combustion chamber (Fig. 1(a)) has been employed. This approach neglects curvature effects from the original RDC geometry, which is justified for this initial study of fundamental 3D detonation structures. The computational domain dimensions (0.1 $m \times$ 0.21 $m \times$ 0.02 m in *x, y*, and *z* directions respectively) correspond to the unwrapped experimental annular combustor [8] with an inner diameter of 0.07 m and a channel width of 0.02 m.

The injection of a premixed stoichiometric kerosene–air mixture is modelled using micro-nozzles, with the injection velocity determined from local pressure conditions, following the methodology of Fievisohn et al. [11]. The simulation employs a linearised channel geometry with periodic boundary conditions, representing an unwrapped annular combustion chamber as shown in Fig. 1. This simplified representation captures the main detonation dynamics while reducing geometric complexity. However, with a diameter-to-width ratio of ~3.5, curvature effects cannot be fully neglected, meaning features such as wave curvature and azimuthal non-uniformities are not fully reproduced. The model should therefore be viewed as an idealised framework to isolate thermal boundary effects. The periodic boundaries enable continuous propagation while accounting for residual combustion products from previous cycles, accurately representing the repetitive nature of detonation wave propagation in RDCs where waves maintain near-constant speed and periodicity.

For boundary conditions, non-reflective outflow is implemented using a characteristic-based formulation to minimise wave reflections, while both inner and outer surfaces are treated as no-slip walls.

The inflow conditions simulate an air-breathing aircraft operating at 25 km altitude with Mach 4.5 flight, yielding total combustion chamber inflow conditions of 7 atm pressure (P_0) and 1000 K temperature (T_0). Initialisation is performed using a Chapman-Jouguet detonation wave to establish physically consistent propagation characteristics throughout the computational domain.

2.3. Simulation cases

Three distinct thermal boundary configurations are investigated, as summarised in Table 1. The case nomenclature follows a logical convention where ’I’ denotes the inner wall, ’O’ the outer wall, ’a’ represents adiabatic conditions, and ’t’ indicates isothermal conditions at 300 K.

Case IaOa serves as the baseline configuration, with both inner and outer walls treated as adiabatic, simulating an uncooled combustor. Case ItOt represents the opposite extreme, where both walls are maintained at a constant 300 K isothermal condition. While 300 K represents an unrealistically low temperature for practical cooling systems (due to the prohibitively large heat sink requirements), this extreme condition is selected to clearly isolate thermal confinement effects. Case IaOt represents an intermediate ’hybrid’ configuration combining an adiabatic inner wall with an isothermally cooled outer wall. This systematic variation of thermal boundaries enables a comprehensive evaluation of confinement effects on detonation wave structures.

Simulations employ a 50 μm uniform grid, satisfying two requirements: (1) being finer than the 50 mm kerosene-air detonation cell size [6], and (2) providing ~ 1000 grids per detonation cell for structural resolution. The 420-million-point mesh advances with $\Delta t = 5 \times 10^{-9}$ s, balancing stability and physical timescale resolution. Calculations were performed on Swansea University’s Supercomputing Wales HPC facility. Seven detonation cycles simulate each case to eliminate initialization effects and reach quasi-steady states.

3. Results and discussion

3.1. Detonation structures confined by adiabatic walls

First, Case IaOa (a detonation wave propagating through the straight-channel RDC confined by adiabatic walls) is analysed. There is no heat transfer through the walls. The wave structures are shown in Fig. 1(b) using the temperature fields. The reactive mixtures of fuel and air are injected from the bottom upward (direction shown by green

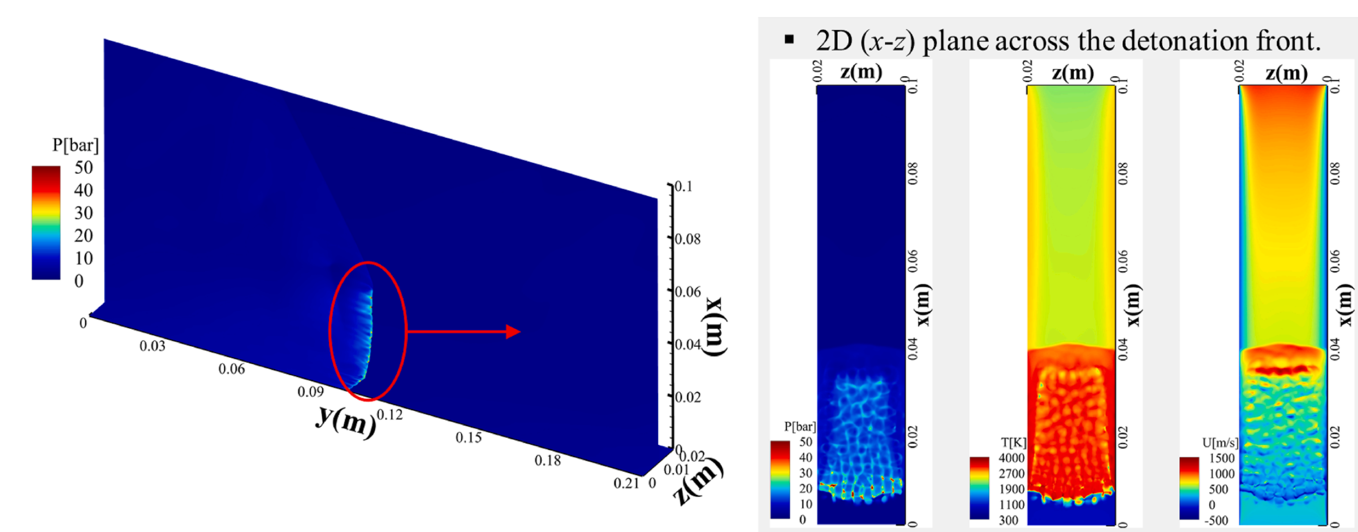

Fig. 2. Instantaneous detonation structures confined by adiabatic walls: Case IaOa.

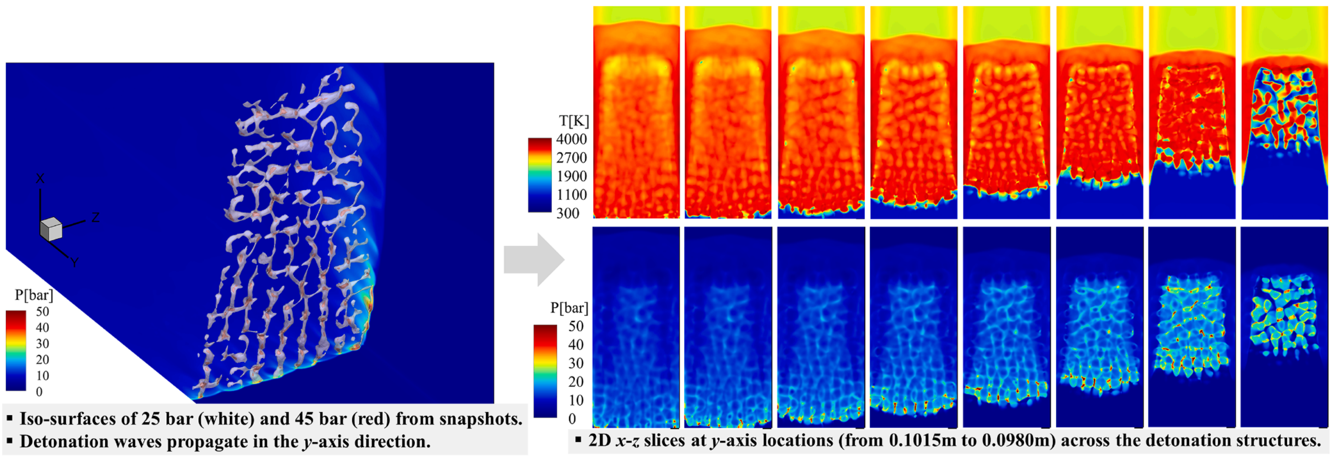

Fig. 3. Iso-surfaces of 25 bar (white) and 45 bar (red) from pressure snapshots of the 3D channel (left) and 2D (*x*-*z*) slices (pressure/temperature distributions) across the curved detonation structures (right): Case IaOa.

arrows), and the detonation wave propagates from left to right. A regular flow structure in the RDC is formed, consisting of an RDW and an oblique shock wave (OSW). From the temperature distribution at the cross-section of the outflow, it is evident that high-temperature boundary layers form near the walls.

The cross-section through the detonation front provides structural analysis, and the distributions of static pressure, static temperature, and velocity in the *x* direction on this 2D cross-section are shown in Fig. 2. In the lower-left part of Fig. 2, a schematic illustrates the thermal conditions of the walls. The distributions of pressure and temperature on the 2D cross-section exhibit the characteristic cellular features of a detonation wave, which cannot be observed from 2D simulations [10]. The width (in the *z*-direction) of the cellular structure narrows as the boundary layer develops along the *x*-direction, affecting the expansion of cellular structures in the channel.

To better understand the detonation structures and elucidate their evolution in the straight-channel RDC, the wave morphology is examined through isosurfaces of static pressure (25 bar and 45 bar), as shown in Fig. 3 (left). These snapshots are extracted from the well-converged phase of the simulation, ensuring they represent sustained propagation behaviour after multiple RDW cycles and are free from initial condition artefacts.

The 3D cellular structure is clearly visible, with detonation kernels (high-pressure red pockets) forming at the intersections of transverse waves (white bandings). These are classified as ’multi-kernels’ since they result from the convergence of more than two transverse waves [1]. Multi-kernels exhibit more extreme thermodynamic states, evidenced by their elevated static pressures.

For spatial evolution analysis, a series of 2D slices along the wave propagation direction (+ *y*) reveals key features of the structures and dynamics, as shown in Fig. 3 (right). Near the channel centre, regular cellular structures with quasi-square lattices dominate, formed by the near-simultaneous intersection of four transverse waves. Moving toward the walls, these features progressively decay due to boundary layer effects, with cellular structures eventually disappearing at the wall interfaces. The self-sustaining propagation mechanism relies critically on the interplay between concave and convex wavefront surfaces within these cellular patterns. This morphological behaviour directly determines the RDW’s ability to propagate continuously, serving as a robust indicator of successful engine operation.

3.2. *Detonation structures confined by isothermal walls*

The analysis turns to cooled-wall configurations, essential for practical engine durability given the extreme temperatures observed in detonation products (Fig. 4). Isothermal walls at 300 K were imposed as an idealised condition selected to maximise thermal gradients, though recognising this represents an extreme case beyond typical cooling system capabilities.

Fig. 4 reveals significant modifications to the detonation structure under cooled boundaries. Along the channel centreline (*x*-*y* plane), a double-wave system emerges, comprising a primary detonation wave

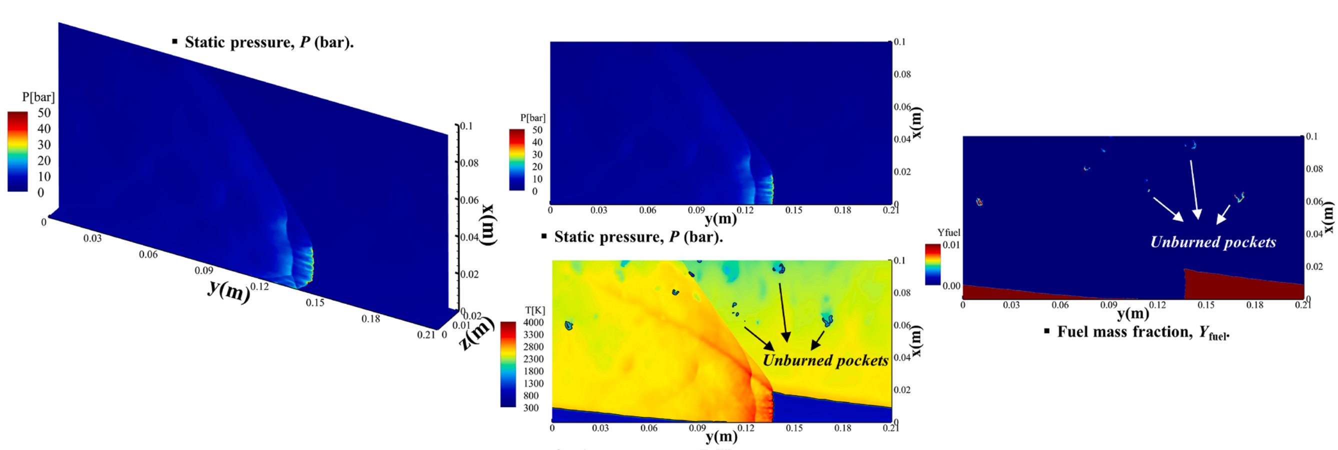

Fig. 4. Detonation structures confined by isothermal walls of 300 K: Case ItOt.

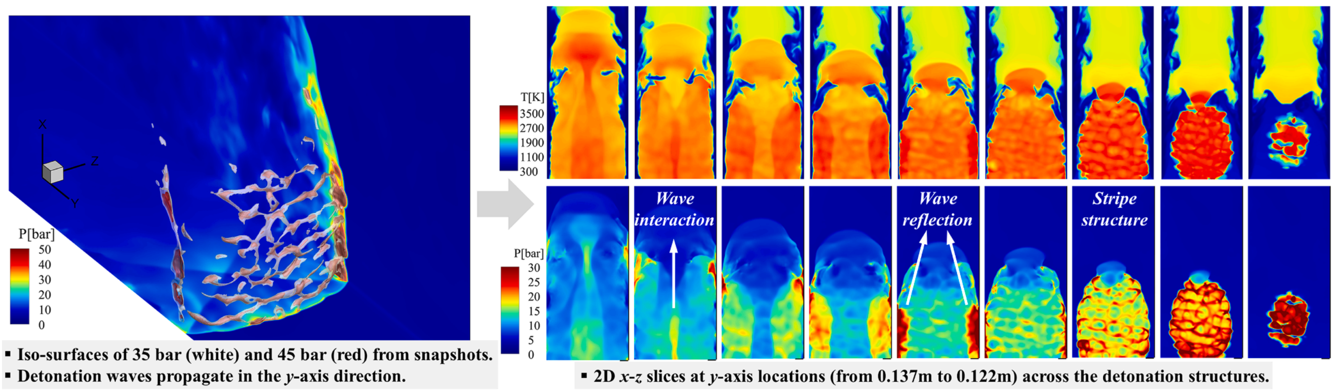

Fig. 5. Iso-surfaces of 35 bar (white) and 45 bar (red) from pressure snapshots of the 3D channel (left) and 2D (*x-z*) slices (pressure/temperature distributions) across the curved detonation structures (right): Case ItOt.

followed by a weaker secondary wave. This contrasts sharply with the single-wave structure of adiabatic Case IaOa, exhibiting a 30–40 % reduction in wave height. The temperature distributions, shown by Fig. 4 (right), further evidence disrupted combustion, with black fuel mass fraction isolines marking substantial unburned pockets and non-uniform reaction zones, compared to the temperature fields for Case IaOa (Fig. 1(b)). The distribution of fuel mass fraction also displays the incomplete combustion in the channel. The cooled walls fundamentally alter wave dynamics through two coupled mechanisms: thermal quenching near boundaries and modified wave interactions. Two detonation waves exhibit divergent angles that drive complex flow field interactions. These changes demonstrate how wall cooling affects detonation propagation at multiple scales - from global wave structure to local combustion completeness.

While the 300 K condition represents an artificial extreme, it provides critical insights for real engine design, highlighting the need for optimised cooling strategies that balance material protection with combustion efficiency.

Building on the methodology applied to adiabatic cases, Fig. 5 (left) presents isosurfaces of static pressure (35 bar and 45 bar) that reveal distinct modifications to detonation structures under cooled-wall confinement. The characteristic stripe-like cellular pattern emerges, dominated by transverse wave bandings (white) aligned preferentially along the *z*-direction before wall collision. This contrasts markedly with the quasi-square lattices observed in adiabatic Case IaOa, where four intersecting transverse waves formed multi-kernels. In the cooled configuration, the reduced wave interactions produce 'line kernels' (red 45 bar pressure spots) at intersections of just two transverse waves.

The evolution of pressure and temperature, captured through sequential 2D slices in Fig. 5 (right), demonstrates three key dynamic processes: First, the leading wave's stripe-like structure expands radially until colliding with the cold boundary layers at the walls, generating intensified reflected waves (evidenced by pressure spikes near boundaries). Second, these reflected waves converge at the channel centre, merging into the secondary wave visible in Fig. 4's *x-y* plane. Third, the continuous wave-wall interactions create significantly more complex transient patterns compared to adiabatic cases, with substantial pressure variations in localised regions near wall collision points.

This analysis reveals how cooled boundaries fundamentally alter detonation physics through two coupled mechanisms: preferential transverse wave alignment and enhanced wave-wall interaction. The resulting structural instability, while potentially challenging for engine operation, provides valuable insights for active cooling system design - particularly regarding the management of reflected wave interactions and secondary ignition zones.

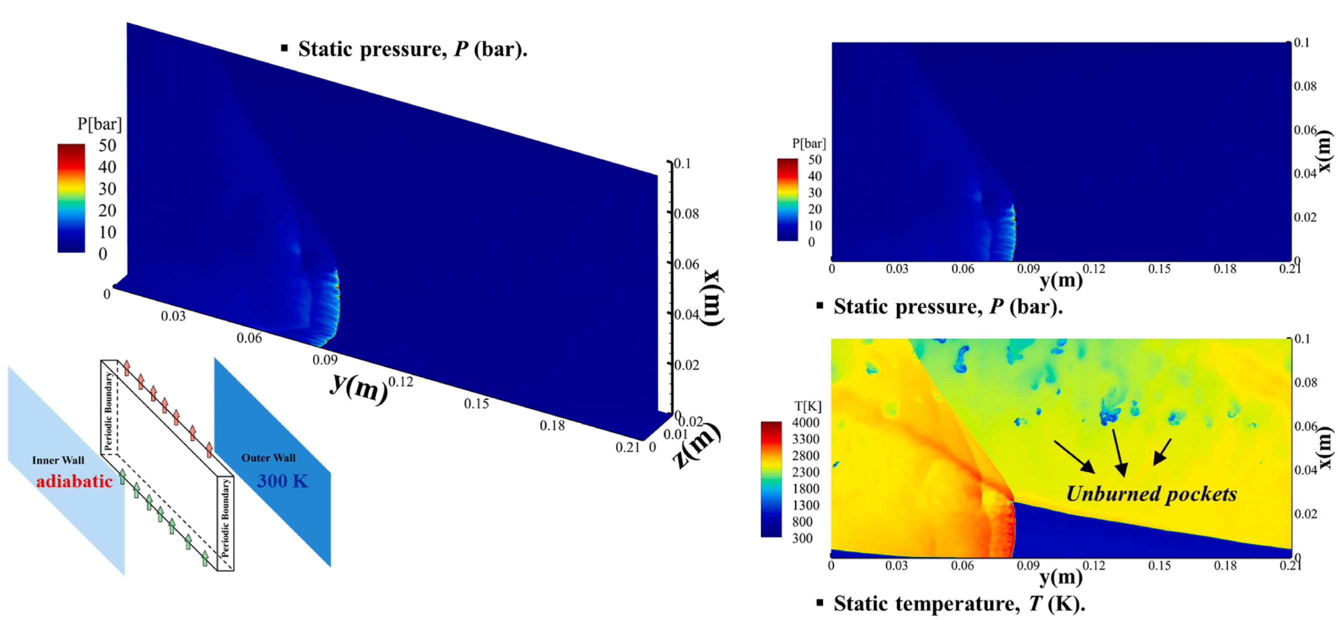

Fig. 6. Detonation structures confined by non-equilibrium thermal walls: Case IaOt.

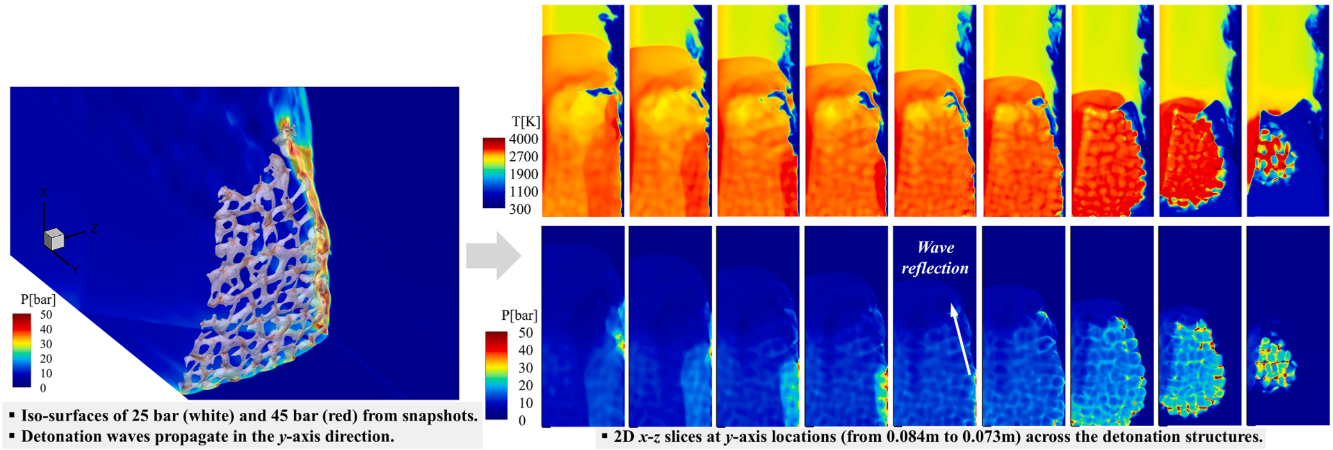

Fig. 7. Iso-surfaces of 25 bar (white) and 45 bar (red) from pressure snapshots of the 3D channel (left) and 2D (*x*-*z*) slices (pressure/temperature distributions) across the curved detonation structures (right): Case IaOt.

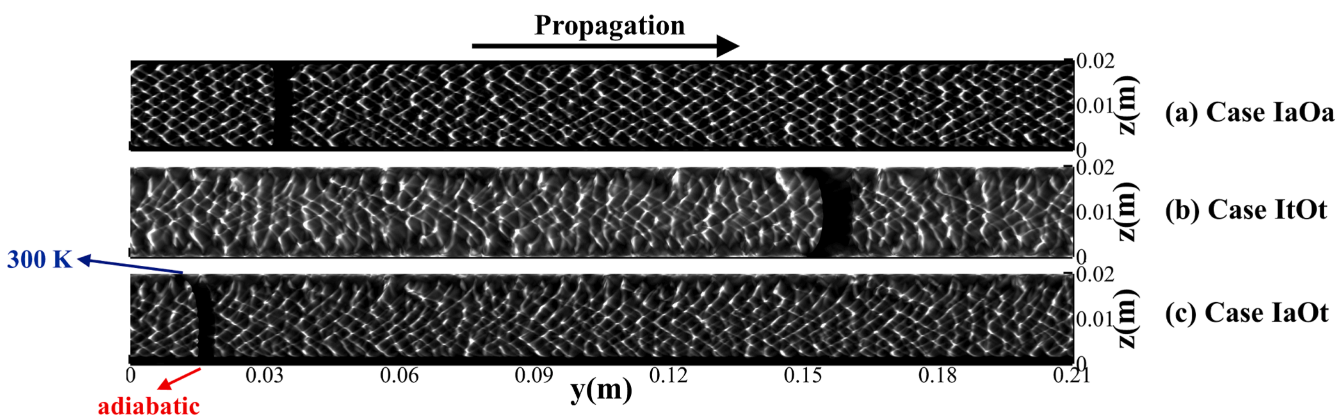

Fig. 8. 2D slice (*y*-*z* cross-section) of 3D maximum pressure history for different thermal confinements: (a) Case IaOa, (b) Case ItOt, and (c) Case IaOt.

3.3. Detonation structures confined by adiabatic wall and isothermal wall

An additional case of detonation structures under asymmetric thermal confinement is studied, where the inner wall remains adiabatic while the outer wall is maintained at a constant 300 K isothermal condition, simulating cooling applied to the outer wall of the RDC (as shown in Fig. 6). Analysis of 2D *x*-*y* planes along the centreline of the channel reveals a pressure field featuring a single detonation front, while the temperature field shows a secondary wave trailing the primary front. Unburned pockets of fuel-air mixtures are visible, demonstrating the persistent effects of partial cooling on combustion completeness.

A snapshot of the pressure isosurfaces is shown in the left part of Fig. 7. As the detonation wave achieves stable self-sustained propagation, its structure (represented by white bandings) closely resembles the quasi-regular pattern observed in Case IaOa. The detonation kernels (visible as red high-pressure spots) represent multi-kernels that connect more than two transverse waves (white bandings). Along the cooled right wall boundary, wave collisions produce a discernible increase in pressure, yet the overall structure maintains characteristic cellular features despite unilateral cooling.

The right part of Fig. 7 displays the dynamic evolution of blast propagation. Each 2D *x*-*z* snapshot features an adiabatic left boundary and a 300 K isothermal right boundary. The rightmost snapshot reveals detonation initiation near the adiabatic wall, attributed to locally elevated temperatures. The front cross-section shows consistent cellular structuring while differing thermal boundaries govern subsequent blast dynamics. Following initiation, the detonation expands toward the cooled wall, with wave strength diminishing due to reactant consumption until wall collision generates an intensified reflected wave. This reflected wave subsequently propagates toward the channel centre, weakening as available reactive mixtures deplete. Compared to the adiabatic side's stable propagation, the cooled boundary induces markedly more dynamic wave behaviour.

3.4. Effects of thermal confinement on detonation structures

The dynamics of cellular structures are analysed based on the maximum pressure history for the straight-channel RDC. The maximum pressure history is derived from full-channel pressure data, representing complete full-scale results. Fig. 8 displays a 2D *y*-*z* cross-section of this pressure history, where black areas correspond to regions where maximum pressure was not tracked. The detonation wave propagation direction runs from left to right across the figure.

Fig. 8 reveals distinct cellular structures under different thermal confinements. The adiabatic boundaries produce more regular detonation cells with consistent sizes compared to those in cooler boundary conditions. While minor deviations occur at the boundaries (Fig. 8(a)), the structure remains highly stable throughout the channel. In contrast, the cold channel with isothermal confinement (Case ItOt, Fig. 8(b)) exhibits irregular structures, evident from random white bandings. These structures show pronounced elongation in the *z*-direction (perpendicular to wave propagation), particularly near the walls. Case IaOt demonstrates intermediate characteristics, combining features from Cases IaOa and ItOt. Near the cold wall, cells stretch in the *z*-direction, while those near the adiabatic boundary maintain more uniform sizing (Fig. 8(c)).

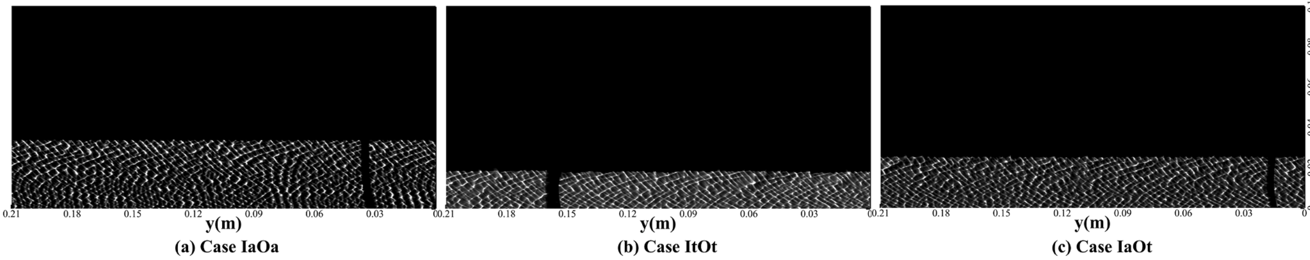

Fig. 9. 2D slice (*x*-*y* cross-section along the centreline of RDC) of the 3D maximum pressure history for identical inflow mixture in different thermal confinements: (a) Case IaOa, (b) Case ItOt, and (c) Case IaOt.

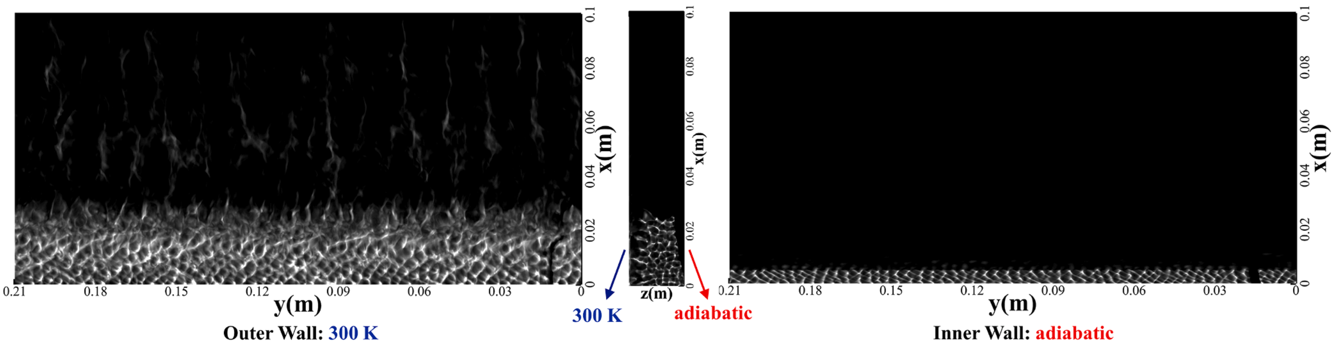

Fig. 10. 2D slides of numerical soot foils for Case IaOt: *x*-*y* cross-section at the inner wall (left), *x*-*z* cross-section across the channel (middle), and *x*-*y* cross-section at the outer wall (right).

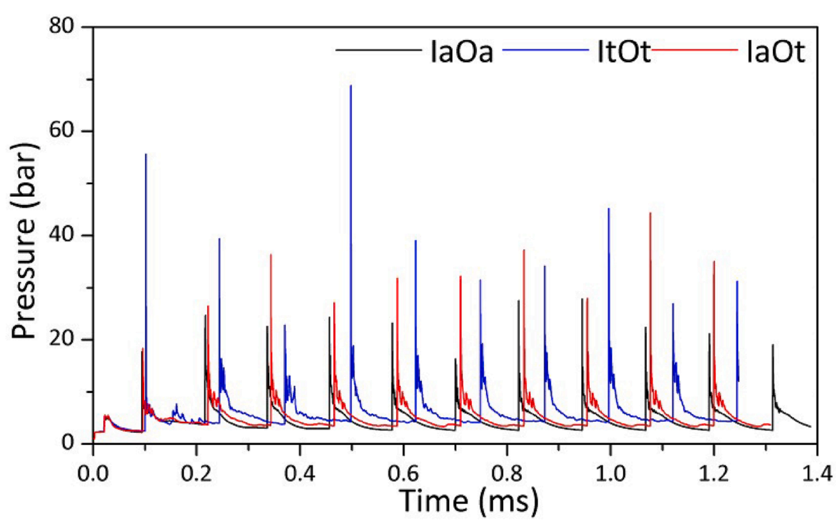

Fig. 11. Pressure signals at an observation point.

Fig. 9 presents complementary 2D *x*-*y* cross-sections along the centreline ($z = 0.01$ m) of 3D maximum pressure history. All cases show characteristic cellular features despite differing wall temperatures. Case IaOa displays the longest detonation wave front (extending to $x \approx 0.03$ m), while Case ItOt produces the shortest. Case IaOt falls between these extremes. The cellular structures remain regular in all cases, though cooling produces slightly narrower *x*-direction cells and elongated *y*-direction cells. This occurs because thermal effects diminish toward the channel centre, furthest from the cooled boundaries.

Fig. 10 provides additional insight into the 3D features of detonation structures by showing the maximum pressure history on both walls with an *x*-*z* cross-section for Case IaOt. The inner wall (right side of Fig. 10) has adiabatic conditions, resulting in regular cellular structures with reduced height near the boundary. This observation is supported by the *x-z* cross-section (middle snapshot in Fig. 10), where the detonation wave height decreases as it approaches the right adiabatic boundary.

On the outer wall side (maintained at 300 K), the cellular structure extends along the *z*-direction while becoming irregular and chaotic. The maximum pressure traces on this isothermal boundary appear as distinct white striations oriented along the x-direction, which are caused by wave-wall interactions. These patterns correlate with the dynamic evolution shown in Fig. 5, demonstrating the complex relationship between detonation waves and walls.

This analysis of Case IaOt (selected due to page limitations) reveals how asymmetric thermal boundaries affect detonation structures: adiabatic walls preserve regularity while cooled walls promote irregularity through wave-wall interactions.

The structural differences in detonation manifest through distinct pressure characteristics among adiabatic, isothermal, and mixed thermal boundary conditions. Pressure signals collected from an observation point (Fig. 11) reveal that the detonation confined by isothermal boundaries (Case ItOt) exhibits the highest peak pressures accompanied by significant instability, characterized by large pressure fluctuations. In contrast, as boundary temperatures increase in Case IaOa (adiabatic boundaries), the pressure rises with fewer fluctuations, primarily because the detonation wave structures remain more stable without strong wave-wall interactions. Case IaOt demonstrates intermediate characteristics, showing decreased pressures relative to Case ItOt along with reduced fluctuation levels. Initially, the detonation under adiabatic boundaries (Case IaOa) propagates fastest, but following an initial transition period, all cases achieve comparable propagation speeds. The most notable difference lies in pressure fluctuation magnitudes - cooled boundaries produce much stronger oscillations due to their lower temperatures.

4. Conclusions

In this work, detailed numerical simulations of detonation wave propagation in a straight-channel combustion chamber were performed, analysing the influence of thermal confinement on the chamber walls. Through analysis of 3D detonation structures and wave dynamics, it was found that:

3D detonation propagation comprises complex shock wave interactions that produce distinct kernel types: line kernels (formed by two intersecting transverse waves) under cooled isothermal conditions, creating stripe-like patterns; and multi-kernels (formed by more than two intersecting transverse waves) under adiabatic confinement, generating regular cellular structures.

Adiabatic confinement produces regular square-lattice structures, whereas cold boundaries induce substantially more complex transverse wave distributions. Cooled chambers develop double-wave structures where wave-wall interactions create extreme thermodynamic states characterised by heightened pressure fluctuations and unburned fuel pockets.

The strong influence of thermal confinements on detonation structure raises important questions about using active cooling to control detonation dynamics.

The conclusions in the present research are found irrespective of the numerical grid resolution used.

Novelty and significance statement

The novelty of this research lies in its detailed exploration of three-dimensional (3D) rotating detonation structures under varying thermal confinements, revealing unique blast dynamics such as stripe-like patterns under cooled boundaries and regular cellular structures under adiabatic conditions. By employing high-fidelity simulations with a kerosene-air mixture, the study uncovers how wall temperatures influence detonation kernels, transverse waves, and unburned pockets—phenomena previously unobserved in 2D or coarse 3D studies. This work is significant because it provides critical insights into the design of cooling systems for rotating detonation combustors (RDCs), addressing practical challenges in thermal management and engine performance. The findings highlight the trade-offs between cooling efficacy and detonation stability, offering a foundation for optimizing RDC operation in propulsion systems. These results advance the understanding of 3D detonation-wave interactions with thermal boundaries, bridging a key gap in combustion science and engineering.

Author contributions

First author’s contributions: designed research, performed research, analysed data, and wrote the paper.

Second author’s contribution: analysed data and revised the paper.

Declaration of competing interests

The authors report no conflict of interest.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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