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Numerical Analysis of the Characteristic Chemical Timescale of a C_2H_4/O_2 Non-Premixed Rotating Detonation Engine

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Abstract: A three-dimensional numerical investigation using ethylene–oxygen was conducted to examine the characteristics of detonation waves in a non-premixed rotating detonation engine (RDE) across three equivalence ratio conditions: fuel-lean, stoichiometric, and fuel-rich. The study aims to identify the distinct timescales associated with detonation wave propagation within the combustor and to analyze their impact on detonation wave behavior, emphasizing the influence of equivalence ratio and injector behavior on detonation wave characteristics. The results indicate that the wave behavior varies with mixture concentration, with the ethylene injector demonstrating greater stiffness compared to the oxygen injector. In lean mixtures, characterized by excess oxidizer, waves exhibit less intensity and slower progression toward equilibrium, resulting in prolonged reaction times. Rich mixtures, with excess fuel, also show a delayed approach to equilibrium and an extended chemical reaction timescale. In contrast, the near-stoichiometric mixture achieves efficient combustion with the highest thermicity, rapidly reaching equilibrium and exhibiting the shortest chemical reaction timescale. Overall, the induction timescale is generally 2–3 times longer than its respective chemical reaction timescale, while the equilibrium timescale spans a broad range, reflecting the complex, rapid dynamics inherent in these chemical processes. This study identifies the role of the characteristic chemical timescale in influencing the progression of pre-detonation deflagration in practical RDEs. Prolonged induction times in non-ideal conditions, such as those arising from equivalence ratio variations, promote incomplete reactions, thereby contributing to pre-detonation phenomena and advancing our understanding of the underlying flow physics.



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Keywords: chemical timescale; ethylene injection; ignition delay; rotating detonation engine (RDE); thermicity

1. Introduction

Rotating detonation engines (RDEs) leverage the power of detonative combustion, offering significant advantages over conventional deflagration-based combustion devices. Detonation is fundamentally a combustion-driven shock that creates a concentrated heat release zone characterized by elevated pressure (p) and temperature (T). Unlike pulse detonation engines [1], RDEs aim to achieve improved efficiency and performance by employing detonative combustion continuously. However, realizing the full potential of RDEs demands a thorough understanding of the complex underlying physics governing non-ideal detonation behaviors. Over the past decade, a substantial body of research has delved into the characteristics of H_2 -based RDEs through both experimental [2–5] and numerical [6–9] studies. However, for practical engine applications, there is a pressing need to transition to more energy-dense, hydrocarbon-based fuels. Among the various

potential alternatives, ethylene (C_2H_4) has emerged as a promising candidate. This is primarily due to its inherently higher detonability compared to most other hydrocarbons, making it more efficient for use in detonation engines. Furthermore, C_2H_4 serves as a crucial intermediate product in high-temperature combustion processes, which further underscores its suitability and potential advantages for RDE applications [10]. One of the primary challenges in utilizing higher hydrocarbon fuels is the inherent low flame speed, which is typically three times lower than that of H_2 [11]. These characteristics hamper the ability to achieve complete combustion within the very brief flow residence time, which is typically on the order of 1 ms.

One of the pioneering reviews on the challenges associated with modeling the multi-scale nature of detonation was conducted by Powers [12]. Wolański [13] explored the RDE timescales linked to modal behavior, providing foundational insights into the dynamics of these systems. Subsequently, Stechmann et al. investigated the blowdown time constant and cycle time using a simplified one-dimensional (1D) model [14]. Fievisohn et al. discussed the timescales pertinent to post-detonation deflagration conditions, shedding light on the transition phases within detonation processes [15]. Bennewitz et al. offered a comprehensive analysis of various timescales relevant to rotating detonation rocket engines (RDREs). Their work provided detailed explanations and quantifications for each timescale, significantly advancing the theoretical framework [16]. Expanding on these first-principle models, Dave et al. employed a case study of the standard RDRE configuration to illustrate the intricate physical processes within experimentally validated RDREs, enhancing the practical understanding of these engines [17]. Further contributions include Wang et al.'s investigation into the ignition time and start-up time of a lab-scale experimental RDE, which provided critical data for optimizing the initiation phases of detonation engines [18]. Burke's detailed examination of RDRE characteristics encompassed various timescales affecting performance including injector design, flame propagation, and control strategies [19]. Additionally, Koch et al. proposed a simplified 1D model using the Euler approach to simulate fluid flow and wave propagation, considering key processes like injection, mixing, combustion, and exhaust, and assigning characteristic timescales to each [20].

RDEs involve a complex interplay of various physical processes, each operating on its own characteristic timescales (τ_c). Understanding these τ_c is crucial for interpreting and optimizing RDE simulations. Figure 1 illustrates a breakdown of major τ_c in RDEs, alongside the ideal Zel'dovich–Neumann–Döring (ZND) structure. These timescales can be broadly categorized based on chemical kinetics, flow/mixing, injector, and acoustics. Chemical timescales, primarily governed by intricate chemical reactions, are instrumental in dictating the fundamental detonation process. The induction time ($\tau_{ind.}$), representing the duration for the fuel–oxidizer mixture to reach critical conditions for detonation initiation, ranging from 0.05 to 1000 ns, and influences the propagation delay and pre-detonation deflagration regions. Pre-detonation deflagration is a critical phenomenon in practical RDEs that arises due to incomplete combustion ahead of the detonation wave. Variations in equivalence ratio (ϕ) and injector dynamics are shown to significantly influence the $\tau_{ind.}$, leading to deflagration regions. To avoid confusion and enhance clarity, it is important to distinguish between ignition delay and $\tau_{ind.}$. Ignition delay refers to the overall time from the initiation of a triggering event, such as fuel injection or heating, to the onset of combustion, encompassing both physical (e.g., vaporization, mixing) and chemical processes. In contrast, the $\tau_{ind.}$ pertains exclusively to chemical kinetics, representing the time required for reactants to reach critical intermediate concentrations and trigger rapid combustion reactions. While these terms may overlap in certain contexts, their differentiation is critical for accurately describing combustion phenomena in this study. The

chemical reaction time ($\tau_{\text{rxn.}}$), reflecting the energy release period of the detonation wave, also spans from 0.05 to 1000 ns, and impacts the heat release rate, and p rise. Additionally, the chemical equilibrium time ($\tau_{\text{eq.}}$), which ranges from 0.001 to 300 ns, influences the post-detonation product composition and T . The chamber residence time ($\tau_{\text{res.}}$), which determines the average duration that fluid particles spend in the chamber, ranges from 0.1 to 10 ms. The reactant mixing time ($\tau_{\text{mix.}}$), referring to the time required for unburned reactants to mix with hot detonation products, also falls within the 0.1 to 10 ms range. Additionally, the available mixing time ($\tau_{\text{avail.}}$), which influences the interaction between the wave and fresh reactants, impacting wave stability and propagation, ranges from 1 to 10 ms. Injection timescales are crucial in the detonation process, particularly in influencing fuel delivery and mixture preparation. The injector recovery time ($\tau_{\text{inj.rec.}}$), defined as the duration for the injector to recover, ranges from 5 to 50 μs and influences the mixture's readiness for detonation initiation. The injector flow reversal time ($\tau_{\text{inj.rev.}}$), representing the time for flow through the injector to reverse direction, also ranges from 5 to 50 μs . Acoustic timescales ($\tau_{\text{acoustic.}}$), related to sound wave propagation, range from 10 to 1000 μs and can potentially affect p fluctuations and detonation stability. Among the multitude of timescales, this paper mainly focuses on the chemical timescales ($\tau_{\text{ind.}}$, $\tau_{\text{rxn.}}$, and $\tau_{\text{eq.}}$) as they govern the fundamental detonation process.

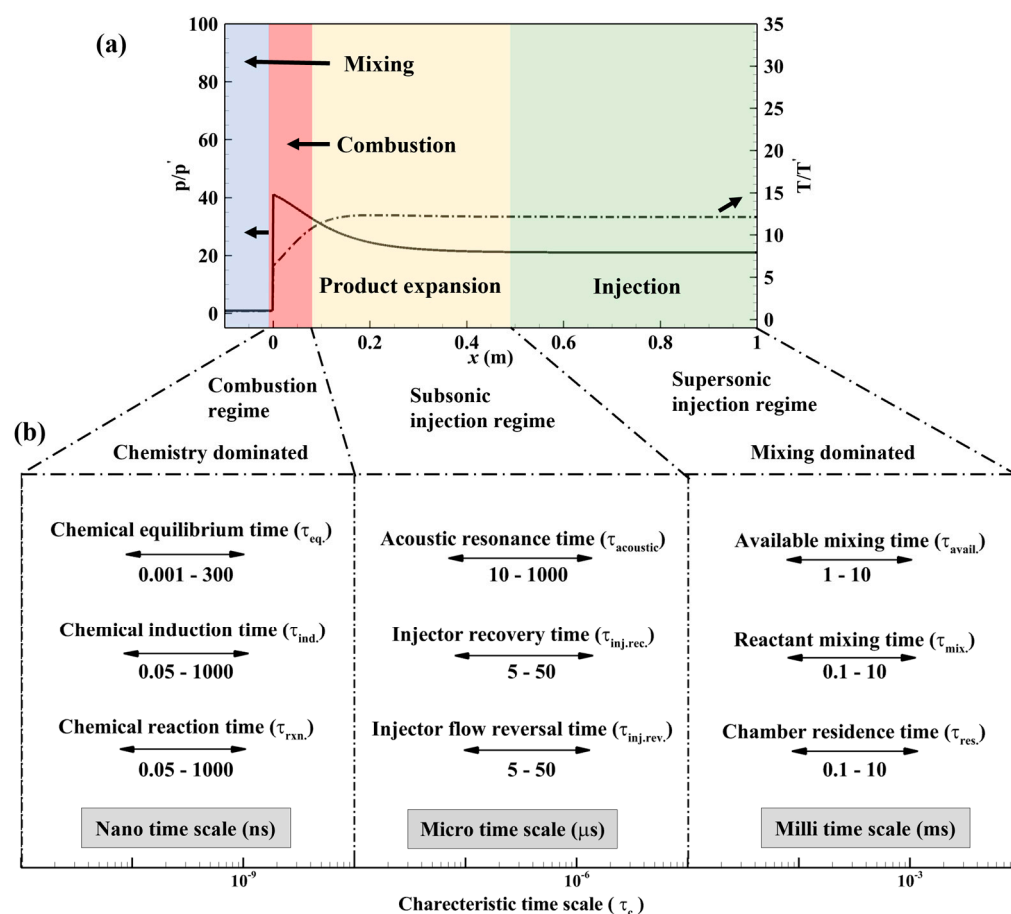


Figure 1. (a) An ideal ZND wave structure with different shaded regions representing combustion (red), product expansion (yellow), injection (green), and mixing (blue). (b) Description of the primary timescale associated with a typical RDE [16].

Figure 2 illustrates the ideal ZND solution for a stoichiometric $\text{C}_2\text{H}_4/\text{O}_2$ mixture at an initial p of 1 atm, highlighting three key chemical timescales. p' denotes the von Neumann pressure, and T' represents the maximum temperature attained at the detonation front. Figure 2a presents the normalized cycle time (t') evolution with respect to p and T , and

Figure 2b gives the mass fraction (Y) of various species. At $t' = 0$ is defined as the point marking the onset of the detonation front location. $\tau_{\text{ind.}}$ is defined as the interval between the characteristic p rise associated with the von Neumann (VN) spike and the moment of maximum heat release, known as the peak thermicity (Θ). In combustion, thermicity refers to the rate of heat release per unit volume due to chemical reactions. It is a crucial parameter for assessing the intensity of energy release within the reaction zone, directly influencing flame stability and propagation. Higher thermicity typically indicates a more vigorous combustion process, impacting flame temperature and overall efficiency. It should be noted that the Θ curve in Figure 2a is presented solely for illustrative purposes; therefore, an additional axis has not been included. $\tau_{\text{rxn.}}$ is defined as the full width at half maximum (FWHM) of the peak Θ curve. This measurement quantifies the duration during which the heat release rate remains at or above 50% of its maximum value. Lastly, $\tau_{\text{eq.}}$ is reached when 99% of the combustion species concentrations (Y_s) attain their Chapman–Jouguet (CJ) state equilibrium values as shown in Figure 2b.

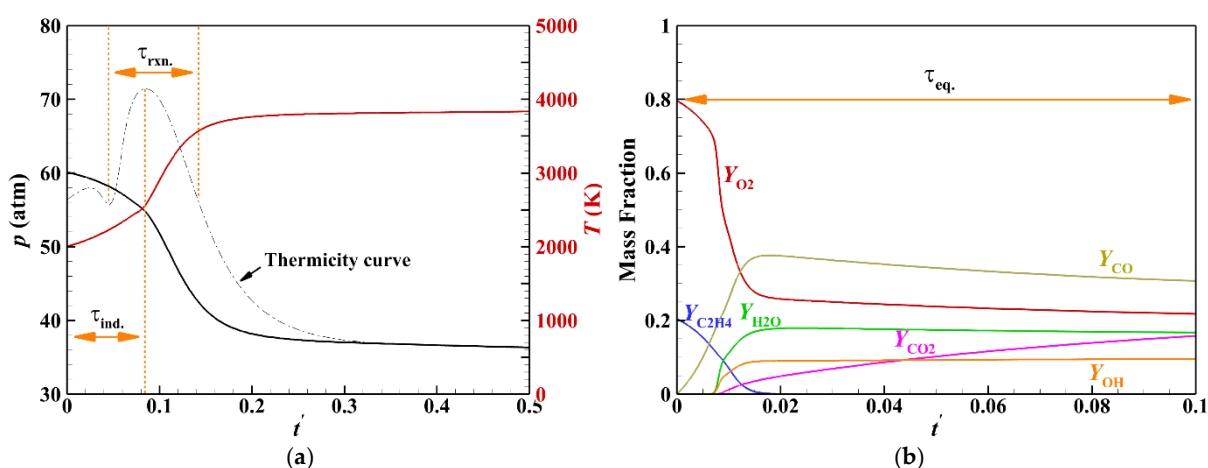


Figure 2. The ideal ZND detonation structure for a $\text{C}_2\text{H}_4/\text{O}_2$ mixture at an ϕ of 1.0 and initial p of 1 atm, showing the normalized temporal evolutions of (a) p and T , and (b) Y_s .

The primary objective of this study is to numerically investigate the behavior of detonation waves in a three-dimensional (3D) non-premixed RDE using ethylene–oxygen mixtures under varying equivalence ratios: fuel-lean, stoichiometric, and fuel-rich. This research focuses on identifying the distinct timescales governing detonation wave dynamics and analyzing their dependence on mixture concentration and injector behavior. The structure of this article is as follows. The subsequent section on numerical methodology provides a detailed overview of the chemical reaction mechanism employed, solver validation, grid convergence analysis, as well as the geometrical configuration and operating conditions of the RDE. The simulation results are then meticulously analyzed and compared, emphasizing the critical findings and insights gleaned from the study. Finally, the article concludes by summarizing the primary outcomes and discussing the broader implications of the research.

2. Numerical Methodology

This study employs an unsteady, fully coupled density-based, compressible, multicomponent 3D reactive flow solver. The governing equations include continuity, momentum, energy conservation, and species composition as given in (1) and (2).

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = \frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + \frac{\partial G_v}{\partial z} + S \quad (1)$$

$$\begin{aligned}
 Q &= \begin{bmatrix} \rho_i \\ \rho u \\ \rho v \\ \rho w \\ e \\ \rho k \\ \rho \dot{\omega} \end{bmatrix} & E &= \begin{bmatrix} \rho_i u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (e + p)u \\ \rho uk \\ \rho u \dot{\omega} \end{bmatrix} & F &= \begin{bmatrix} \rho_i v \\ \rho vu \\ \rho v^2 + p \\ \rho vw \\ (e + p)v \\ \rho vk \\ \rho v \dot{\omega} \end{bmatrix} & G &= \begin{bmatrix} \rho_i w \\ \rho wu \\ \rho wv \\ \rho w^2 + p \\ (e + p)w \\ \rho wk \\ \rho w \dot{\omega} \end{bmatrix} \\
 E_v &= \begin{bmatrix} -\rho_i u_i^d \\ \sigma_{xx} \\ \sigma_{xy} \\ \sigma_{xz} \\ \beta_x \\ \mu_k \partial k / \partial x \\ \mu_{\dot{\omega}} \partial \dot{\omega} / \partial x \end{bmatrix} & F_v &= \begin{bmatrix} -\rho_i v_i^d \\ \sigma_{yx} \\ \sigma_{yy} \\ \sigma_{yz} \\ \beta_y \\ \mu_k \partial k / \partial y \\ \mu_{\dot{\omega}} \partial \dot{\omega} / \partial y \end{bmatrix} & G_v &= \begin{bmatrix} -\rho_i w_i^d \\ \sigma_{zx} \\ \sigma_{zy} \\ \sigma_{zz} \\ \beta_z \\ \mu_k \partial k / \partial z \\ \mu_{\dot{\omega}} \partial \dot{\omega} / \partial z \end{bmatrix} & S &= \begin{bmatrix} S_i \\ 0 \\ 0 \\ 0 \\ 0 \\ S_k \\ S_{\dot{\omega}} \end{bmatrix}
 \end{aligned} \quad (2)$$

where u , v , and w are the velocity vectors in the x , y , and z directions. Total density, ρ , is expressed as the sum of the partial density, ρ_i , of each species as follows:

$$\rho = \sum_{i=1}^{N_s} \rho_i \quad (3)$$

Assuming the ideal gas law for a thermally perfect mixture and the equation of state is given by

$$p = \sum_{i=1}^{N_s} \frac{\rho_i}{M_i} RT \quad (4)$$

where R and M are the universal gas constant and the molecular weight of the i -th species, respectively. The total energy per unit volume (e) is calculated by adding the kinetic energy and internal energy.

$$e = \frac{(u^2 + v^2 + w^2)}{2} + \sum_{i=1}^{N_s} \left(\int \frac{c_{p,i} - R}{M_i} dT + h_i \right) \quad (5)$$

where h_i and $c_{p,i}$ are the enthalpy and the specific heat capacity at constant pressure of the i -th species, respectively, and are given by

$$\frac{h_i}{RT} = \sum_{n=0}^4 \frac{a_{n,i} T^n}{n+1} + \frac{a_{5,i}}{T} \quad (6)$$

$$\frac{c_{p,i}}{R} = \sum_{n=0}^4 a_{n,i} T^n \quad (7)$$

where $a_{n,i}$ with $n = 1 \sim 5$ are the coefficients for the i -th species.

The Wilke formula [21] is used to calculate the dynamic viscosity of the mixture. The thermodynamic properties of each species are evaluated from JANAF polynomials [22]. The thermal conductivity of the mixture is obtained from [23]. This computation integrates the higher-order Monotonic Upstream-centered Scheme for Conservation Laws (MUSCL) for the computation of convective fluxes to enhance the accuracy of capturing sharp gradients. For diffusion fluxes, a second-order central differencing scheme is implemented, providing a balanced approach to handling diffusive terms. Temporal discretization is achieved using a second-order time-accurate fully implicit time integration method. A Courant–Friedrichs–Lewy (CFL) value of 0.5 was uniformly selected across all cases to ensure

numerical stability. The computational solver was parallelized using the Message Passing Interface (MPI) library on shared memory processors to simulate the chemically reacting flow of a 3D non-premixed RDE. Each simulation was executed on nodes equipped with Intel Xeon Gold 6154 CPUs, each featuring 36 cores operating at a frequency of 3.0 GHz.

2.1. Quasi-Global (QG) Chemistry

A quasi-global chemistry mechanism developed by Singh et al. [24] has been utilized for this study, which has been shown to effectively account for the critical dissociation reactions [25]. Table 1 details the mechanism, which comprises 10 steps and 8 reacting species. The rate of these reactions is given by the equation below:

$$R = AT^n \exp(E/RT) \quad (8)$$

Table 1. The quasi-global reaction mechanism for C₂H₄/O₂ system ^a [24].

No.	Reaction ^b	Pre-Exponential Factor (A)	Exponent of T (n)	Activation Energy (E)
1	C ₂ H ₄ + O ₂ ⇌ 2CO + 2H ₂	1.80 × 10 ¹⁴	0.00	35,500
2	CO + O ⇌ CO ₂ + M	5.30 × 10 ¹³	0.00	−4540
3	CO + OH ⇌ CO ₂ + H	4.40 × 10 ⁰⁶	1.50	−740
4	H ₂ + O ₂ ⇌ OH + OH	1.70 × 10 ¹³	0.00	48,000
5	H + O ₂ ⇌ OH + O	2.60 × 10 ¹⁴	0.00	16,800
6	OH + H ₂ ⇌ H ₂ O + H	2.20 × 10 ¹³	0.00	5150
7	O + H ₂ ⇌ OH + H	1.80 × 10 ¹⁰	1.00	8900
8	OH + OH ⇌ H ₂ O + O	6.30 × 10 ¹³	0.00	1090
9	H + H ⇌ H ₂ + M	6.40 × 10 ¹⁷	−1.00	0.00
10	H + OH ⇌ H ₂ O + M	2.20 × 10 ²²	−2.00	0.00

^a Units are in seconds, moles, cm³, calories, and degrees Kelvin. ^b Third-body efficiencies for all thermolecular reactions are 2.5 for M = H₂, 16.0 for H₂O, and 1.0 for all other M.

This mechanism was validated using an extensive array of available shock-tube experimental data [26–31]. Analytical calculations of ignition delay times were conducted for the QG mechanism [24] and the USC Mech II detailed chemistry [32] utilizing the Shock and Detonation Toolbox [33] integrated with Cantera [34]. Figure 3 illustrates the comparison between the predicted ignition delay and the corresponding experimental data, demonstrating the reliability and consistency of the employed mechanism.

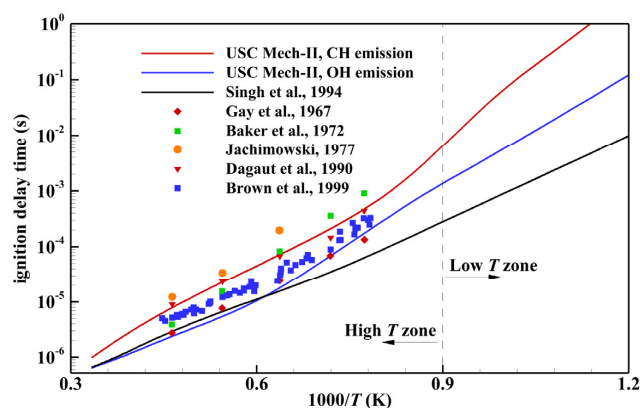


Figure 3. Comparison of ignition delay times with experimental and analytical results.

2.2. Validation

Given the high computational costs associated with 3D analysis, solver validation was conducted through a two-dimensional (2D) analysis using an $\text{H}_2/\text{O}_2/\text{Ar}$ mixture. Simulations focusing on planar detonations within a straight channel are employed to characterize cellular structures formed during the detonation process.

The computational domain, as depicted in Figure 4a, with dimensions of 7 cm in height and 120 cm in length. The grid size is uniformly set to $\Delta x = \Delta y = 25 \mu\text{m}$. The chamber is filled with a premixed mixture of $\text{H}_2/\text{O}_2/\text{Ar}$ at a chamber p of 0.06 atm and a chamber T of 298 K. The left boundary is configured with a slip wall condition, while the right boundary is set with zero gradient. Cyclic boundary conditions are applied to the top and bottom walls. The detonation wave is initiated by introducing a high-pressure region near the left boundary. This region has an ignition p of 25 times higher than chamber p and an ignition T that is 6 times higher than chamber T . A comparative analysis of results from both the present solver, as shown in Figure 4b, and the study by Wang et al. (Figure 4c) reveals a comparable cell size of approximately $57 \times 32 \text{ mm}$ and $54 \times 30 \text{ mm}$, respectively. The cellular structures comparing both cases exhibit a higher degree of consistency. Further validation is provided in Figure 5, which juxtaposes the cell width under varying initial p at stoichiometric with the findings of Strehlow et al. [35].

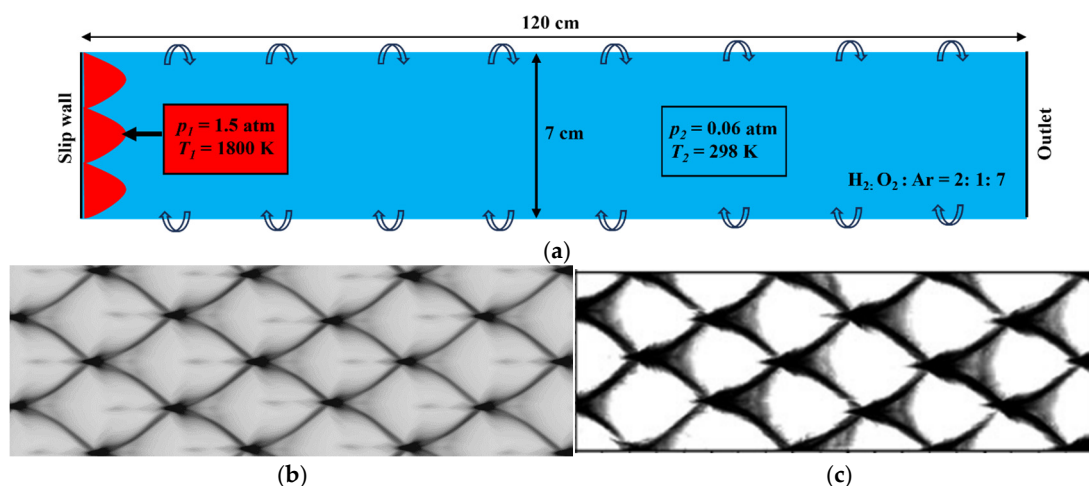


Figure 4. (a) 2D computational domain for planar detonation. (b) Cell structure predicted by the current solver and (c) by Wang et al. [36].

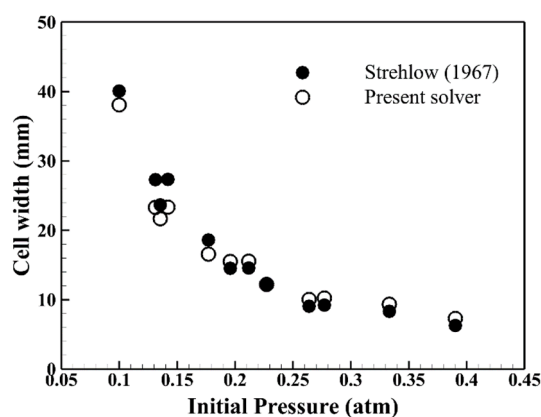


Figure 5. Comparison of cell width with varying initial p by the present solver and Strehlow et al. [35].

2.3. Geometrical Configuration

The geometrical configuration utilized in this study is a 2.3-inch diameter-based RDE conducted at the Pusan National University (PNU) [37,38]. Figure 6a shows the complete computational geometry, offering an overview of the entire simulation domain. Figure 6b focuses on the computational mesh in the near-injector field, highlighting the grid resolution. Figure 6c zooms in on the inlets for C_2H_4 and O_2 , including a 30° supersonic expansion throat and the backward-facing step (BFS). To ensure adequate distance for the dissipation of p waves exiting the detonation chamber without reflective interference back into the chamber, the simulation domain has been expanded beyond the initial experimental geometry. The post-detonation plenum is characterized by a limited number of computational cells to facilitate the numerical dissipation of waves. This design mirrors many previous cross-flow RDE configurations [7,8]. Unlike H_2 -based RDEs, this configuration features a wider annulus to accommodate the relatively slower C_2H_4/O_2 chemistry. Fuel is introduced into the detonation chamber through 47 individual square-type injector ports, each with an inlet area of 1 mm^2 . The oxidizer is introduced circumferentially via a narrow slit with a width of 0.5 mm . The detonation chamber has an inner diameter of 50 mm , an outer diameter of 59 mm , and an annulus thickness of 4.5 mm . The height of the detonation chamber measures 75 mm . The entire computational domain is partitioned into 517 sub-domains to facilitate MPI parallel simulation. Figure 6d illustrates the arrangement of the computational blocks associated with only two of the C_2H_4 injectors. Table 2 provides a comprehensive summary of the simulation cases performed in this study.

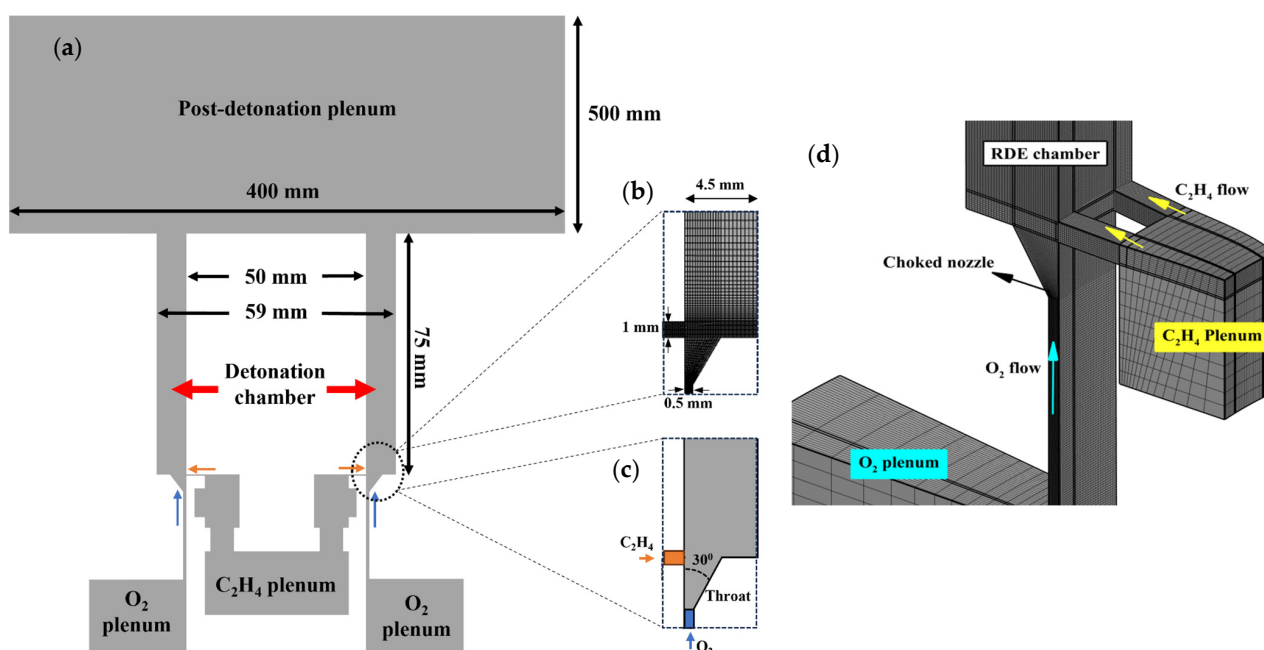


Figure 6. (a) The computational geometry; (b) computational mesh in the near-injector region; (c) a close-up view of the inlets; and (d) two-injector multi-block grid system for RDE.

Table 2. Details of the simulation cases for the C₂H₄/O₂ reaction system.

Parameters	RDE Chamber (Initial Conditions)	Fuel-Lean Mixture ($\phi = 0.9$)		Near-Stoichiometric Mixture ($\phi = 1.01$)		Fuel-Rich Mixture ($\phi = 1.1$)	
		Case 01		Case 02		Case 03	
		C ₂ H ₄ Plenum	O ₂ Plenum	C ₂ H ₄ Plenum	O ₂ Plenum	C ₂ H ₄ Plenum	O ₂ Plenum
Mach	0.01	choked		choked		choked	
T_0 (K)	300	300		300		300	
P_0 (atm)	1.973	2.269	3.792	2.305	4.116	2.549	5.311
O ₂ mixture (%)	75	-	100	-	100	-	100
C ₂ H ₄ mixture (%)	25	100	-	100	-	100	-

2.4. Grid Convergence

For the grid-convergence test, four different structured grids were used. The baseline mesh has a resolution of 1.2×10^{-4} m, resulting in a total of 16.6 million control volumes (MM) within the detonation chamber. This baseline mesh is determined by conducting analytical induction length calculations for stoichiometric C₂H₄/O₂ detonations under similar conditions. With this baseline mesh as a reference, a series of simulations were conducted using coarse, fine, and very fine meshes. The resolutions for the coarse, fine, and very fine meshes are 1.56×10^{-4} m (8.23 MM), 0.84×10^{-4} m (33.21 MM), and 0.588×10^{-4} m (65.35 MM), respectively. To accurately capture the detonation waves propagating near the chamber base-head, the grid resolution in the near-injector region is made significantly finer compared to the downstream sections of the chamber. Specifically, a uniform fine resolution is maintained up to 30% of the chamber height from the bottom across all meshes to accurately capture the detonation waves. Beyond these near-field regions, the remaining chamber area is assigned a coarser grid, with the resolution twice the initial fine resolution. This approach balances computational efficiency with the need for detailed simulation, optimizing the trade-off between accuracy and computational cost. The simulation was conducted with slip conditions applied to the side walls and a zero-gradient condition applied to the exhaust outlet.

The temporal evolution of p and T probe data extracted from a location near the injector head is compared for all grid cases, as illustrated in Figure 7a. The coarse mesh exhibits a deviation in p and T by approximately 0.1 atm and 50 K, respectively. This deviation is primarily due to numerical diffusion and the presence of unreacted pockets. As the mesh resolution increases, these deviations progressively diminish. In the fine and very fine grid resolutions, the differences become almost negligible. Furthermore, a comprehensive investigation was conducted to examine the convergence of errors in the VN peak p (p_{VN}) and detonation wave speed (ω) relative to the finest resolution ($\Delta x = 0.588 \times 10^{-4}$ m), as depicted in Figure 7b. The results reveal a consistent convergence in p_{VN} with increasing grid resolution. In contrast, ω displays a more complex relationship with grid resolution. This is attributed to the intricate dynamics of species evolution within the detonation wave, resulting in non-monotonic convergence patterns. Despite these complexities, it is noteworthy that even at the coarsest resolution, the error in ω remains below 1%, indicating that the simulations maintain a high degree of accuracy across different grid resolutions.

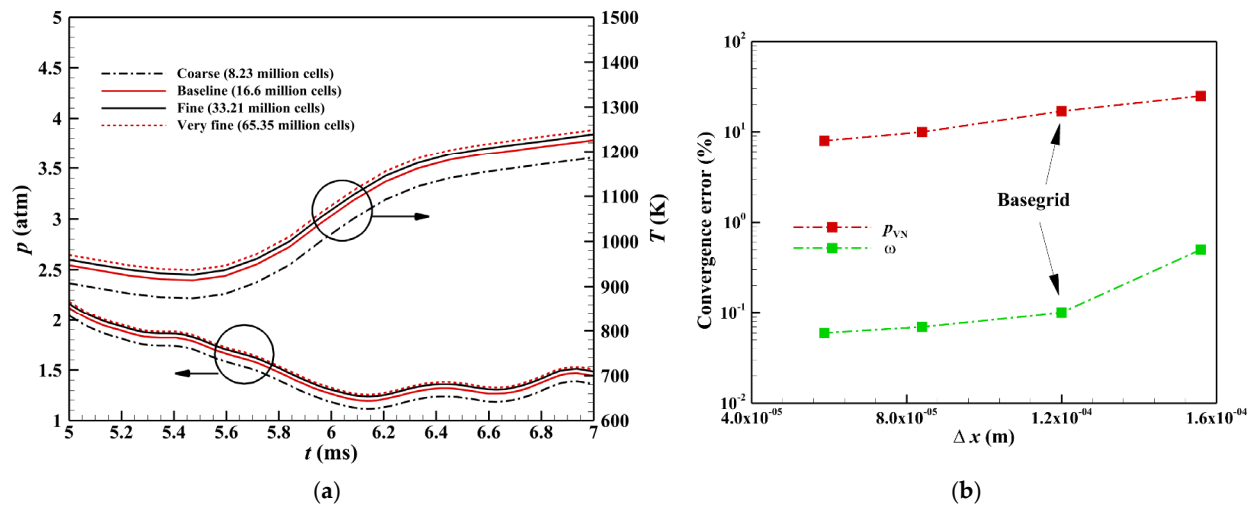


Figure 7. (a) Probe data illustrating the temporal evolution of p and T profiles, and (b) error convergence of p_{VN} and ω with grid sizing.

3. Results and Discussion

3.1. Macroscopic Flow-Field Comparison

Figure 8 displays the instantaneous p contour from a top view, taken from an axial cut situated 2% above the BFS for each grid configuration. Here, a self-sustained detonation wave was observed across all grid configurations. The coarse and baseline grids exhibit higher numerical diffusion, resulting in multiple unreacted pockets and a larger post-detonation region. This leads to a less accurate representation of the wave structures, although it is computationally less demanding. In contrast, the fine and very fine grids significantly improve the resolution quality, revealing the most detailed features of the detonation waves. As the mesh resolution increases, the wavefronts become progressively clearer, the p gradients are more accurately captured, and the shock waves appear sharper.

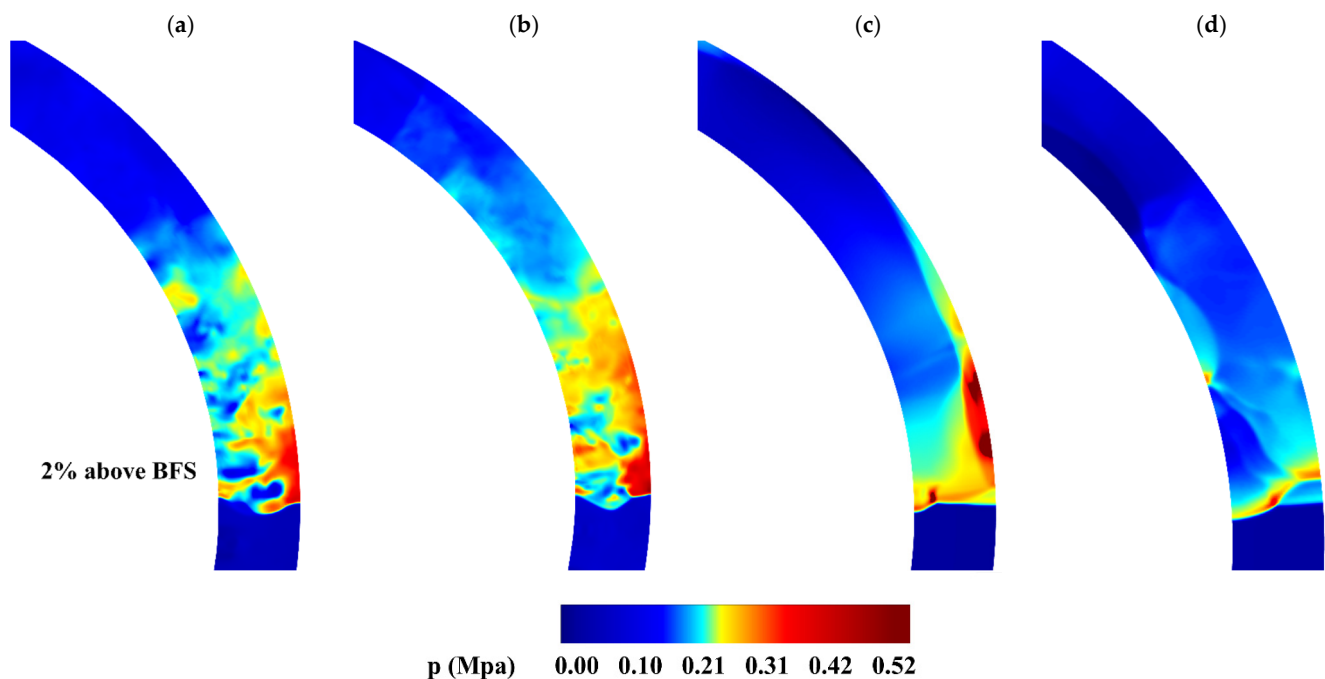


Figure 8. Instantaneous p field of the RDE using different resolution meshes: (a) coarse, (b) base, (c) fine, and (d) very fine mesh cases.

3.2. Instantaneous Flow-Field

After reaching steady-state operation, a single wave began to develop in the azimuthal direction, driving the coalescence of existing p waves and fast flames. Eventually, waves propagating in the anticlockwise direction prevailed, establishing a stable rotating wave. A rendered visualization of these rotating waves is presented in Figure 9, where the iso-contour pressure profile clearly depicts the detonation front, its propagation direction, post-detonation mixing, and fuel/oxidizer injection. The region behind the detonation front exhibits unburned reactant pockets, labeled as “e”, which clearly demonstrate the presence of incompletely combusted reactants. This suggests a significant likelihood that incoming reactants are not entirely consumed by the detonation front and are instead carried along behind the advancing wave. These unburned reactant pockets indicate potential inefficiencies in the combustion process, where a portion of the reactant mixture bypasses the primary combustion zone. This phenomenon could influence the stability and overall energy release of the detonation, as the unburned reactants may contribute to secondary combustion events or interact with other flow structures downstream.

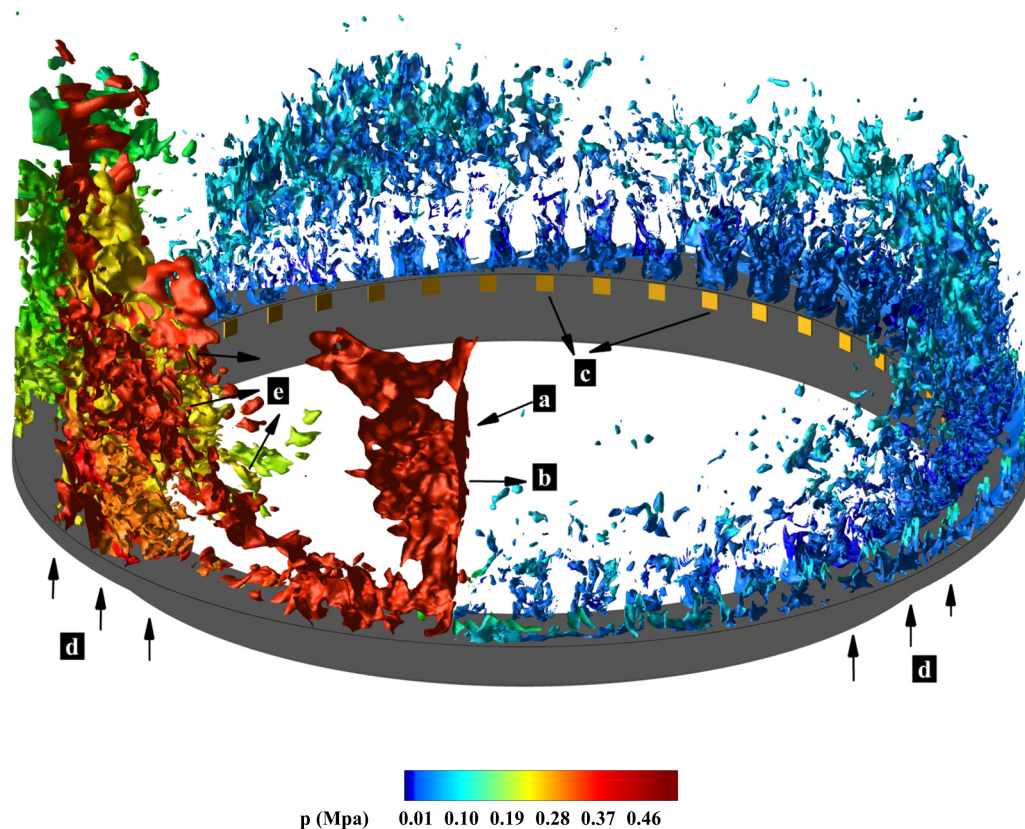


Figure 9. Three-dimensional view of a single anti-clockwise detonation wave under steady-state operation, highlighting the injection process. The illustrated isocontours are colored by pressure. The nomenclatures are (a) detonation wave, (b) moving direction, (c) discrete C_2H_4 injector, (d) slit O_2 injector, and (e) unburned pockets.

Figure 10 presents instantaneous snapshots of the p contours within the RDE annulus. These figures depict the contours on the outer wall, mid-channel, and a cutting plane located 2 mm above the BFS for fuel-lean, near-stoichiometric, and fuel-rich cases, respectively. In all three cases, the numerical solver effectively captures key flow field features such as the self-sustained detonation front, oblique shocks, and slip lines. On a macroscopic level, significant differences are observed in detonation behavior such as variations in detonation height, the angle of the oblique shock, the vertical detonation front, and p

propagation back to the plenum. For the fuel-lean case, the outer-wall p indicates a less intense wave, resulting in a less vigorous reaction suggesting that the wavefront is broader and less defined. In the near-stoichiometric case, the outer-wall flow field shows a more intense and sharper gradient, indicating a more powerful and efficient detonation. In the fuel-rich case's outer-wall p shows additional diffusion and mixing, with a more dispersed wavefront. The flow field observed at the mid-channel, in contrast to the outer wall, exhibits a more stratified structure. This stratification can be primarily attributed to two factors: Firstly, incomplete displacement of product gases by freshly re-filled gases results in weaker detonations. As new fuel and oxidizer mixtures enter the chamber, they do not fully displace the existing product gases, leading to areas where the detonation process is less intense. This incomplete displacement can cause fluctuations in the flow field properties, contributing to the stratified nature. Secondly, the use of discrete injectors introduces the reactants in such a way that creates pockets of varying composition throughout the flow field. This non-uniformity hinders the formation of a homogeneous mixture, which is essential for a consistent and powerful detonation front. As a result, the flow field in the mid-channel remains stratified, with regions of differing reactant concentrations and detonation strengths. In the mid-chamber, the fuel-lean case exhibits a front that is slightly elevated from the chamber bottom, likely due to incomplete mixing at the bottom. Conversely, the near-stoichiometric case shows a reduced wave height, appearing attached to the bottom wall, indicating more complete combustion. The fuel-rich case displays a slightly less defined wavefront compared to the other cases.

Examining the cut sections, the post-detonation strength in the fuel-lean case is relatively lower, with the wave spreading out more diffusely and showing less pronounced inner and outer wall gradients. The near-stoichiometric mixture exhibits a stronger post-detonation strength, with the wave spreading more uniformly and displaying greater compression closer to the outer wall. The fuel-rich mixture case shows moderate post-detonation strength, with a less defined wavefront and more gradual gradients along the inner and outer walls compared to the near-stoichiometric case. Specifically, the high p region in the post-detonation zone expands with increasing fuel levels. This observation suggests a significant influence of expansion effects as the detonation propagates through the curved channel of the RDE. Such behavior aligns with the findings of Frolov et al. [39], who identified similar phenomena in their studies. The forward azimuthal slant indicates that the detonation wave interacts dynamically with the curved geometry of the combustion chamber, leading to differential propagation speeds between the inner and outer walls.

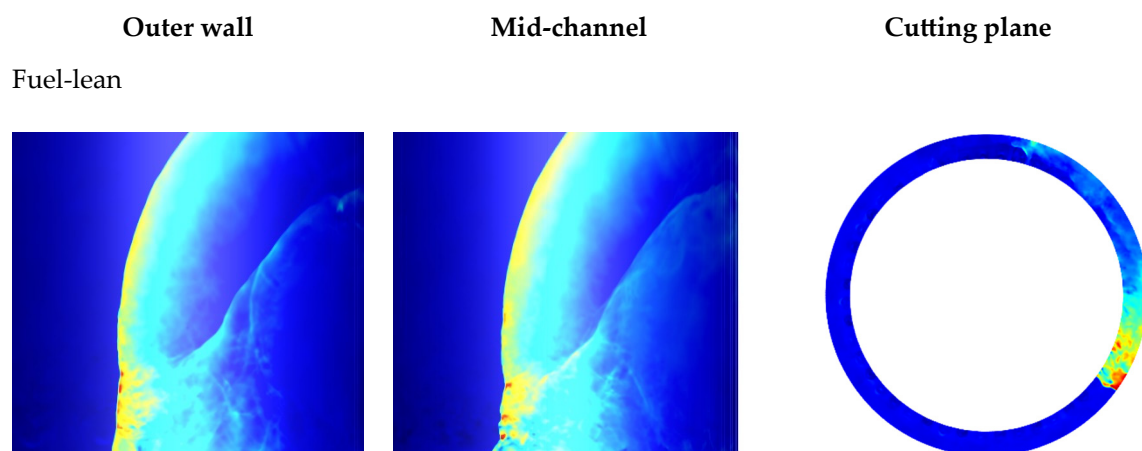
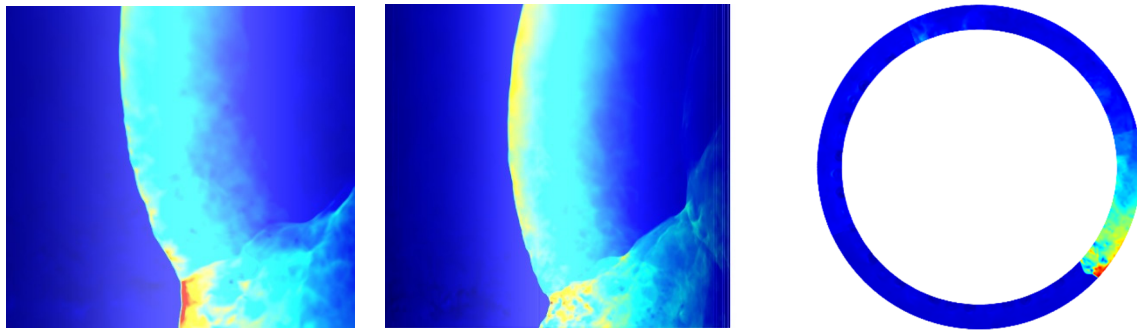


Figure 10. Cont.

Near-stoichiometric



Fuel-rich

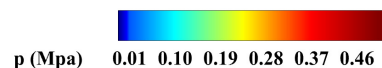
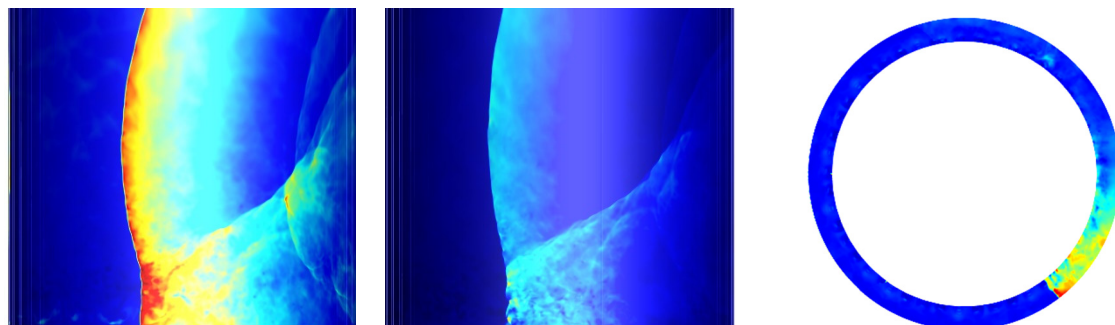


Figure 10. Instantaneous p field with different case studies; fuel-lean, near-stoichiometric, and fuel-rich. Outer wall (**left-column**), mid-channel (**middle-column**), and a cutting plane (**right-column**).

3.3. Axial Pressure Distribution

A quantitative assessment and validation have been carried out by comparing numerical simulations with corresponding experimental data [38]. Figure 11 illustrates the axial pressure for the fuel-lean, near-stoichiometric, and experimental cases with error bars. The x -axis zero point corresponds to the bottom head of the detonation chamber. The uncertainty in the simulations was estimated by considering multiple factors, including numerical discretization errors, grid resolution effects, and sensitivity to input parameters such as boundary conditions and thermochemical properties. The resulting uncertainty was quantified by calculating the standard deviation across these variations. The results indicate that the numerical simulations align well with the experimental data across all cases. Near the chamber bottom, the results show relatively higher pressures, suggesting active mixing processes. As the detonation wave progresses downstream, the product gases expand towards the exit, resulting in a gradual decrease in pressure. There is a notable variation between fuel-lean and near-stoichiometric cases. At $\phi = 1.01$, there is improved mixing, more complete combustion, and fewer unreacted pockets, which leads to higher pressure.

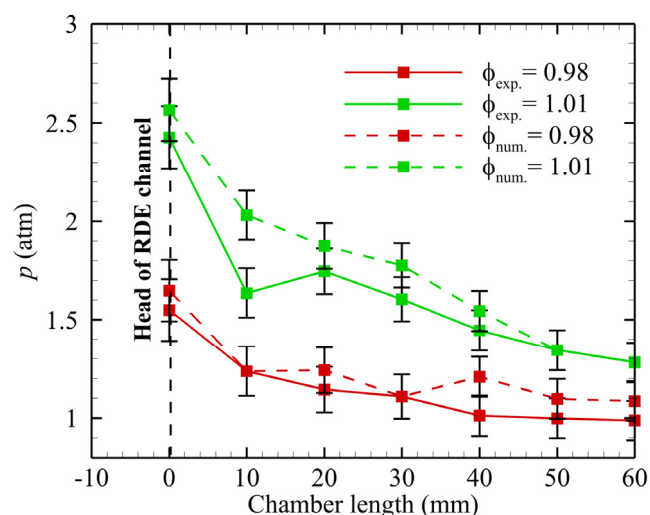


Figure 11. Comparison of outer body wall pressure along the RDE length.

3.4. Injector Flow Profiles and Its Dynamics

To comprehensively analyze the flow characteristics in relation to the detonation front, three distinct slices were extracted. Figure 12 presents a 2D line diagram showing the slice locations within the computational domain. In the figure, the detonation front moves from right to left. Only 70% of the chamber's axial height is depicted here and in the subsequent figures because no significant variations occur beyond this point. Slice-1, located ahead of the detonation front, offers insights into the flow dynamics before the onset of detonation. Slice-2 is positioned at the detonation front, providing detailed information on the structure of the wave and the immediate reaction zone. Slice-3 examines the post-detonation flow features.

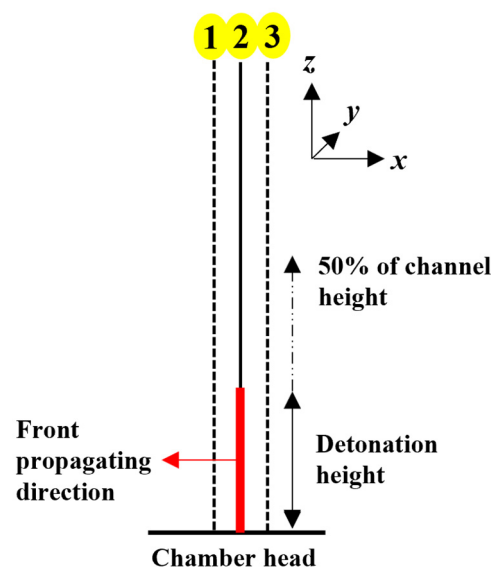


Figure 12. 2D line diagram depicting the locations of axial–azimuthal slices.

Figure 13 presents axial–azimuthal slices of the instantaneous Y_{O_2} near the injector, highlighting the complex interactions between the injected fuel and the surrounding O_2 . Figure 13 (left) presents the fuel-lean mixture case. In the pre-detonation slice, there is a clear distinction between C_2H_4 and O_2 concentrations. The C_2H_4 stream is pushed into the chamber due to the axially incoming O_2 from the bottom. Efficient mixing primarily occurs at three locations: (1) at the intersection between the C_2H_4 and O_2 streams, (2) at a certain distance from the chamber bottom, and (3) near the outer wall, likely due to

recirculation in this area. This trend is consistent with findings reported by others [40–42], highlighting similar mixing behaviors in detonation chambers. Additionally, the O_2 stream impacts the outer wall at the BFS, creating a mode-locked lean layer near the outer wall. This phenomenon is notable as the O_2 inlet provides a continuous 360° inflow, while the C_2H_4 injectors are discrete. The on-detonation wave slice depicts the formation of reaction zones and the beginning of combustion. As combustion initiates, the reactant concentration decreases, and the formation of multiple small reactant pockets can be seen, reflecting its consumption in the reaction process. The presence of a prominent pressure wave (represented by a white line) overlaid on top shows the detonation wave. In the post-detonation slice, minimal C_2H_4 concentration is observed, as the slice is taken between two C_2H_4 injectors. Clear evidence of combustion products moving downstream can be noted.

Figure 13 (middle) presents near-stoichiometric conditions. In the pre-detonation slice, it is evident that the amount of C_2H_4 interacting with the outer wall is higher compared to the fuel-lean case. In the BFS area, there is an absence of complete mixing of reactants, resulting in a region predominantly filled with O_2 . The fresh reactant mixture moves upstream to approximately 12% to 15% of the chamber height, highlighting the extent of C_2H_4 penetration and mixing. In the on-detonation wave slice, the presence of the C_2H_4 mixture remains significantly higher at the front compared to the fuel-lean case, indicating a dominance of C_2H_4 . The efficient mixing of reactants and the subsequent combustion process are clearly observed. The pressure gradient shows the strength of the detonation front, likely close to the injector head. In the post-detonation slice, the contours show a predominance of O_2 , likely due to the injector fuel primarily moving axially upstream rather than radially. The supersonic incoming O_2 speed likely overtakes the radially spreading C_2H_4 speed, further pushing the C_2H_4 upstream. The rapid downstream movement of combustion products is also significantly higher, indicating robust and efficient combustion.

Figure 13 (right) presents the fuel-rich mixture. In the pre-detonation slice, the quantity of incoming C_2H_4 is significantly higher compared to the other cases. As the fuel progresses downstream, distinct layers of more diffused stoichiometric mixing become evident. However, due to the increased availability of reactants, the diffusion process becomes more widespread. The fresh reactant mixture advances upstream up to about 15% to 20% of the detonation height. In the on-detonation wave slice, combustion has initiated and taking place; however, many unreacted pockets are still visible, indicating incomplete combustion. The concentration of the C_2H_4 mixture remains notably higher at the outer wall, suggesting a less efficient mixing and reaction process. In the post-detonation slice, the C_2H_4 concentration moves axially upstream and azimuthally due to the higher initial fuel concentrations. Numerous unreacted pockets are still visible, highlighting areas where the combustion process has not fully completed affecting the overall efficiency and performance of the detonation process.

The mixing process in RDE systems is inherently chaotic, primarily due to the non-premixed discrete cross-flow injection. This complexity arises not only from the separate injection of fuel and oxidizer but also from the phenomenon of injector blocking or flashback caused by the detonation wave propagating through the chamber. When the detonation wave passes, it temporarily blocks the injector, necessitating a recovery period before the refilling process can resume. This dynamic behavior varies with changes in mixture concentration, further complicating the understanding of RDEs. Therefore, it is crucial to thoroughly assess the injection dynamics over a complete cycle for both the fuel and oxidizer injectors. Figure 14 presents probe data for the U , p , and Y_s at the injector location for both fuel and oxidizer inlets, plotted as a function of t' . By normalizing t with respect to the total cycle duration, the figure effectively highlights the temporal variations in injection properties within a single cycle.

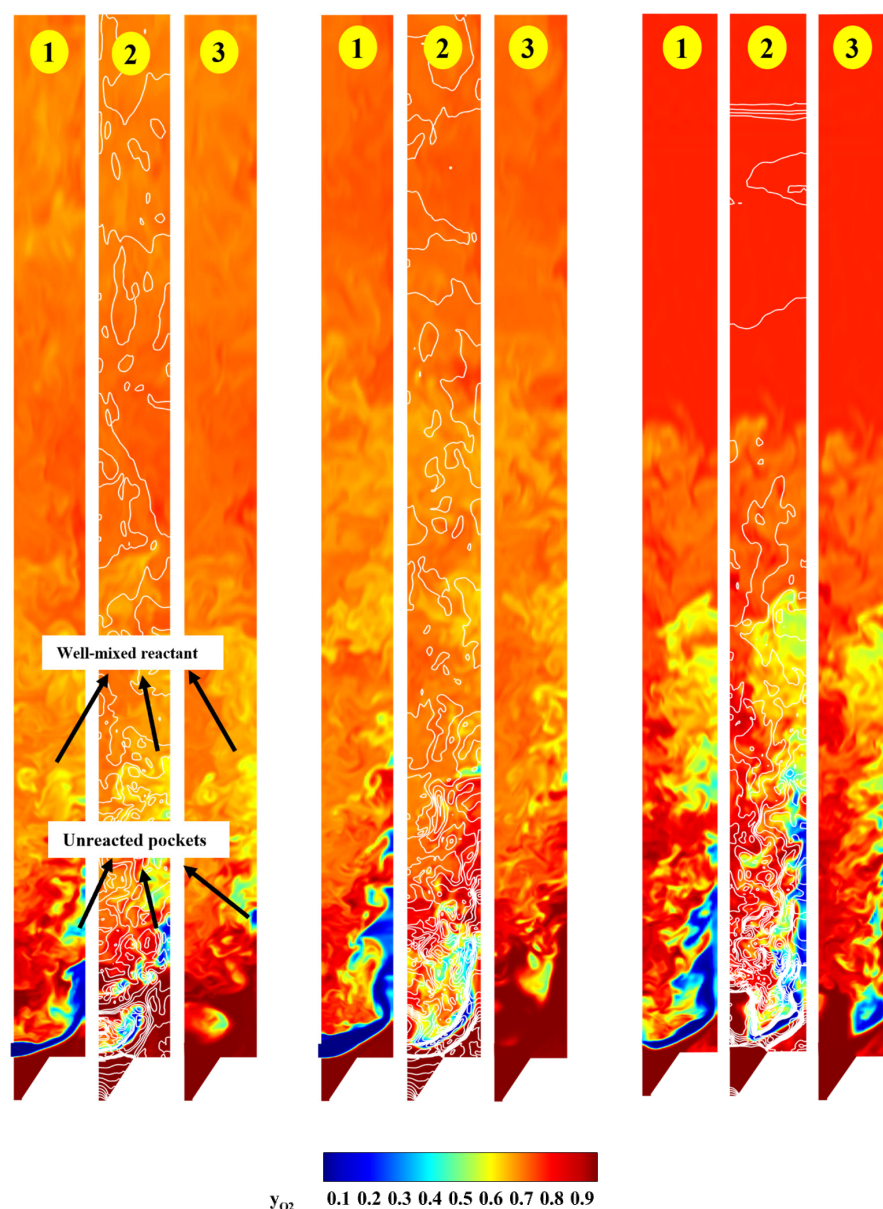


Figure 13. Instantaneous Y_{O_2} mixture along the axial–azimuthal slices: (1) pre-detonation, (2) at the detonation front, and (3) post-detonation for (left) fuel-lean mixture, (middle) near-stoichiometric mixture, and (right) fuel-rich mixture.

As shown in Figure 14a,b, a sudden drop in injection U at $t' = 0.22$ – 0.41 (approx.) indicates that both fuel and oxidizer injectors are obstructed as the detonation wave passes. At the C_2H_4 injector, this U drop is more pronounced with a rapid recovery for the fuel-lean case. In contrast, for the fuel-rich mixture, the U drop is less severe, and the flow recovery is slower. Similar flashbacks are also observed for O_2 injection, though their dynamics differ slightly from those of the C_2H_4 injector. The U drop for the O_2 injection is significantly stronger because it is positioned directly below the detonation waves, whereas the fuel injector is located at the cross-section of the wave. Here, the pattern shows that the flow tends to tumble for a period before gradually recovering to its original value, consistent with observations from previous studies on non-premixed RDEs. Notably, the C_2H_4 injector exhibits stiffer behavior compared to the O_2 injector, highlighting the more pronounced response and recovery patterns in the O_2 injection process. Examining the p profiles presented in Figure 14c,d reveals several key observations. Firstly, the p spike is significantly higher for the stoichiometric case at both injectors, indicating a more intense

detonation wave within the chamber. Secondly, the p spike at the C_2H_4 injector is nearly half that observed at the O_2 injector. This disparity suggests that the O_2 injector, being directly beneath the detonation wave, experiences a more substantial impact. Thirdly, post-detonation fluctuations are prominently visible at the O_2 injector, with almost two-thirds of the chamber experiencing disturbances before the arrival of fresh reactants. In contrast, these post-detonation effects are scarcely noticeable at the fuel injectors. The Y_s profiles for both fuel and oxidizer are depicted in Figure 14e,f, respectively. The distinct recovery phases and differing trajectories highlighted illustrate the intricate mixing processes occurring within the chamber. This complexity contributes to the formation of a highly chaotic detonation structure. These variations underscore the challenges in achieving uniform mixing and highlight the intricate nature of the detonation wave propagating within the combustion chamber.

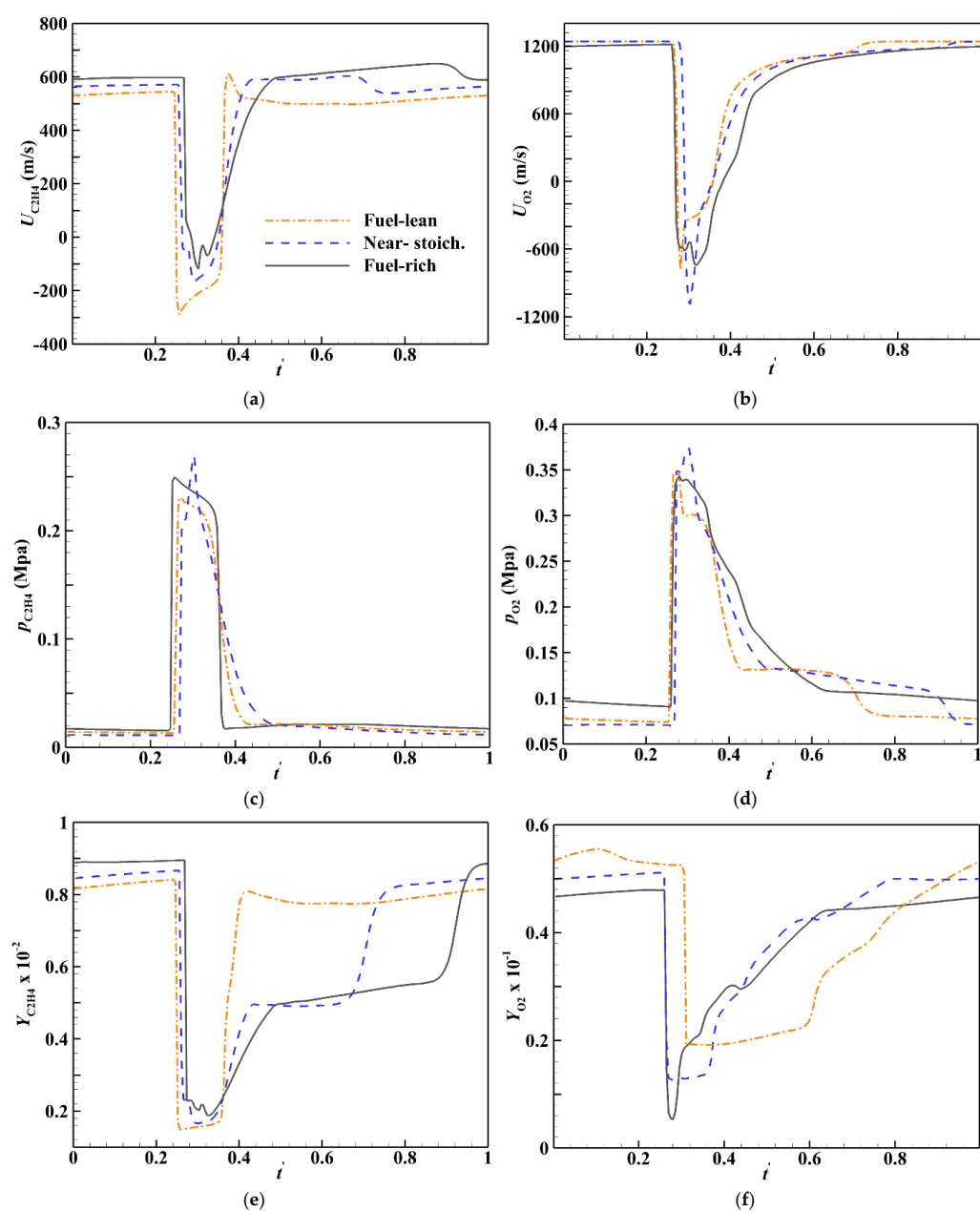


Figure 14. Variation in injection parameters showing (a) $U_{C_2H_4}$, (b) U_{O_2} , (c) $p_{C_2H_4}$, (d) p_{O_2} , (e) $Y_{C_2H_4}$, and (f) Y_{O_2} with cycle-averaged time for (left-column) fuel and (right-column) oxidizer.

3.5. Chemical Reaction Timescale

This section investigates the τ_{rxn} associated with three distinct mixture cases. Figure 15 shows the shock-normal averaged profiles of p and T . The left y -axis represents normalized p (instantaneous p normalized by p_{VN} of the lean mixture), while the right y -axis represents normalized T (instantaneous T normalized by the maximum T of the lean mixture). The x -axis denotes t' , and the blue line illustrates Θ across the various mixtures. Once again, it should be stressed here that the Θ curve in the figure is presented solely for illustrative purposes; therefore, an additional axis has not been included.

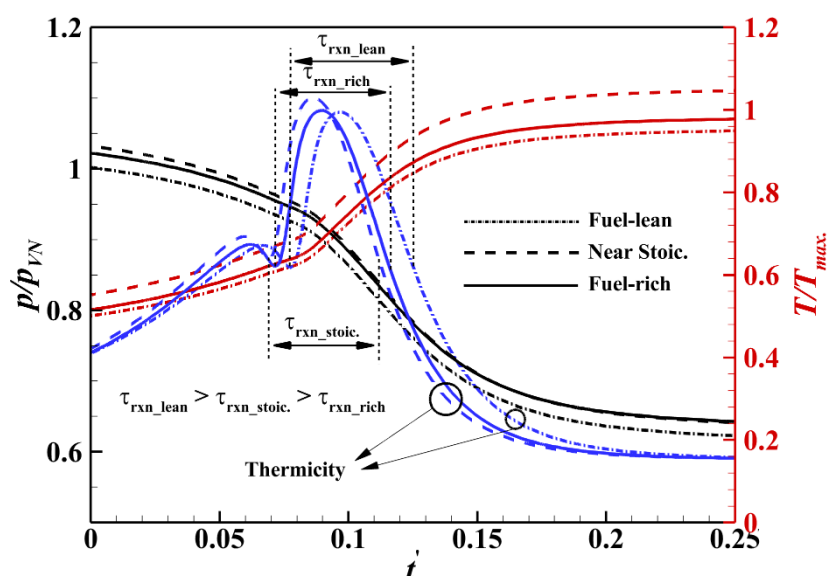


Figure 15. Variation in τ_{rxn} plot across different ϕ .

First of all, it has become evident that the 1D detonation structure profile calculated using CJ assumptions in ZND models, deviates markedly from the structure profiles obtained from multi-dimensional detonation simulations. Several factors contribute to these significant discrepancies, including the presence of discrete injectors, varying chemical timescales, incomplete mixing, parasitic combustion, and the expansion of product gases. Flow properties are measured across the wavefront at the mid-channel, at a specific height above the injector near-head, to examine this time scale.

The lean mixture exhibits relatively lowest Θ , p/p_{VN} , and T/T_{max} , indicative of a less intense detonation front. The near-stoichiometric mixture shows the highest Θ reflecting the most intense and effective detonation wave, signifying the most efficient combustion. The rich mixture, on the other hand, falls in between the lean-mixture category and the near-stoichiometric category. Equilibrium is reached most quickly in a near-stoichiometric mixture, as evidenced by the rapid stabilization of both p/p_{VN} and T/T_{max} . The rich mixture requires more time to achieve equilibrium, while a lean mixture takes even longer. This disparity is attributed to the slower reaction kinetics due to the presence of excess oxidizer and fuel, which result in the formation of unreacted pockets. The lean mixture, characterized by an excess of oxidizer, exhibits less intense wave behavior and a slower approach to equilibrium, leading to prolonged reaction times. The rich mixture, which has an excess of fuel, also shows a slower approach to equilibrium and longer τ_{rxn} . Conversely, the near-stoichiometric mixture, with optimal fuel-oxidizer balance, displays the highest Θ , achieves the most efficient combustion, reaches equilibrium the fastest, and has the shortest τ_{rxn} among all the mixtures.

3.6. Chemical Induction Timescale

Figure 16 demonstrates $\tau_{ind.}$ for three distinct mixtures, utilizing the same plot and nomenclature described in Figure 15. The induction zone, which marks the onset of significant chemical reactions, critically influences the structure, propagation speed, and stability of the detonation wave, exhibiting notable variations among the three cases. In the lean mixture, the induction zone appears notably prolonged, indicating a slower initiation of chemical reactions. This extended duration can be attributed to the excess O_2 content, which reduces overall reactivity and delays the buildup of radicals essential for sustained combustion. Consequently, the mixture requires more time to achieve the critical conditions necessary for rapid exothermic reactions. This delay is evident in the extended time required to reach peak Θ , accompanied by a more gradual p/p_{VN} decline and a less abrupt $T/T_{max.}$ increase. The near-stoichiometric mixture displays a compact induction zone characterized by a swift increase in Θ , accompanied by a rapid elevation in p and T , signifying the presence of a robust and stable detonation wave. This mixture promotes effective radical formation and accelerates chain branching reactions, resulting in a shortened induction time that facilitates prompt chemical reactions, thereby maximizing the rate of energy release. Comparatively, the rich mixture, although outperforming the lean counterpart, still exhibits a longer induction time than the near-stoichiometric mixture. Notably, the induction time is typically around 2–3 times longer than their respective $\tau_{rxn.}$. In the near-stoichiometric mixture, peak Θ occurs rapidly, aligning with the brief induction time, indicating rapid energy conversion critical for sustaining a robust detonation wave. The rich mixture, on the other hand, experiences a delayed peak Θ , corresponding to their longer induction times and less efficient heat release processes. Analysis of the $\tau_{ind.}$ reveals a strong correlation between prolonged induction times and the onset of pre-detonation deflagration. In lean and rich mixtures, the chemical reactions proceed more slowly due to non-optimal fuel-oxidizer ratios. This delay fosters localized deflagration regions ahead of the detonation wave.

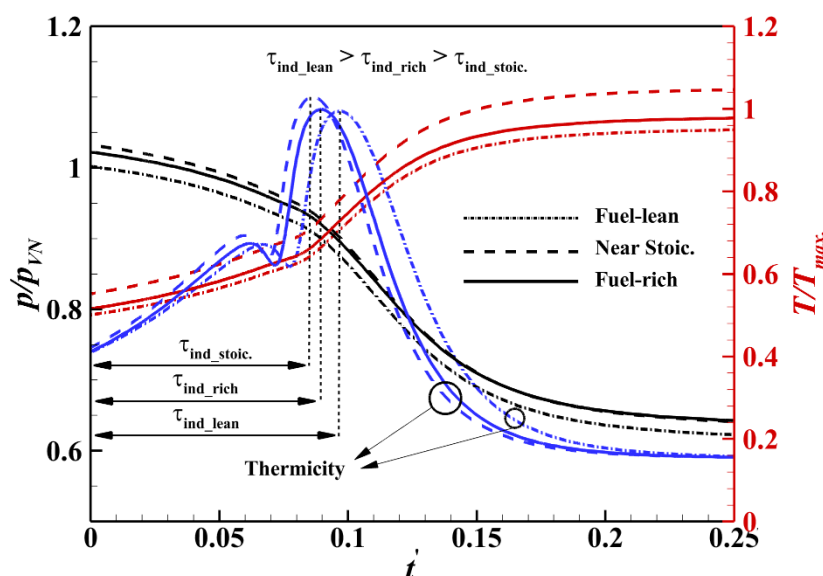


Figure 16. Variation in $\tau_{ind.}$ plot across different ϕ .

3.7. Chemical Equilibrium Timescale

This section examines the formation of four critical species OH, CO, C_2H_4 , and O_2 due to their substantial impact on combustion properties. It is important to note that the timescales presented here for these species should not be extrapolated to other species generally. Figure 17 illustrates the $\tau_{eq.}$ for three distinct mixtures for four different species. As illustrated in Figure 17a, Y_{OH} varies significantly across different mixtures, influencing

the combustion characteristics. In lean mixtures, the excess O_2 undergoes further decomposition due to the ample availability of O_2 molecules to form hydroxyl radicals, resulting in higher OH fractions. These higher OH levels enhance reactivity. Conversely, in rich mixtures, the insufficient O_2 leads to lower OH fractions, resulting in faster reaction rates that reach equilibrium more quickly. The near-stoichiometric mixture demonstrates optimal fuel-oxidizer mixing, achieving the most efficient combustion with minimal unburned residues. Figure 17b reveals that $\tau_{eq.}$ for the Y_{CO} differs significantly from Y_{OH} . In rich mixtures, higher CO fractions are observed due to excess fuel, but it takes a longer time to reach chemical equilibrium. Lean mixtures, with excess O_2 , show lower CO fractions as more CO is oxidized to CO_2 or forms hydroxyl radicals, leading to rapid species formation and faster equilibrium compared to fuel-rich mixtures. The near-stoichiometric mixture maintains a moderate CO fraction and equilibrium time. Similarly, Figure 17c,d provides $\tau_{eq.}$ for $Y_{C_2H_4}$ and Y_{O_2} . Overall, the $\tau_{eq.}$ spans a broad range of timescales, highlighting the variability and rapid dynamics in these chemical processes.

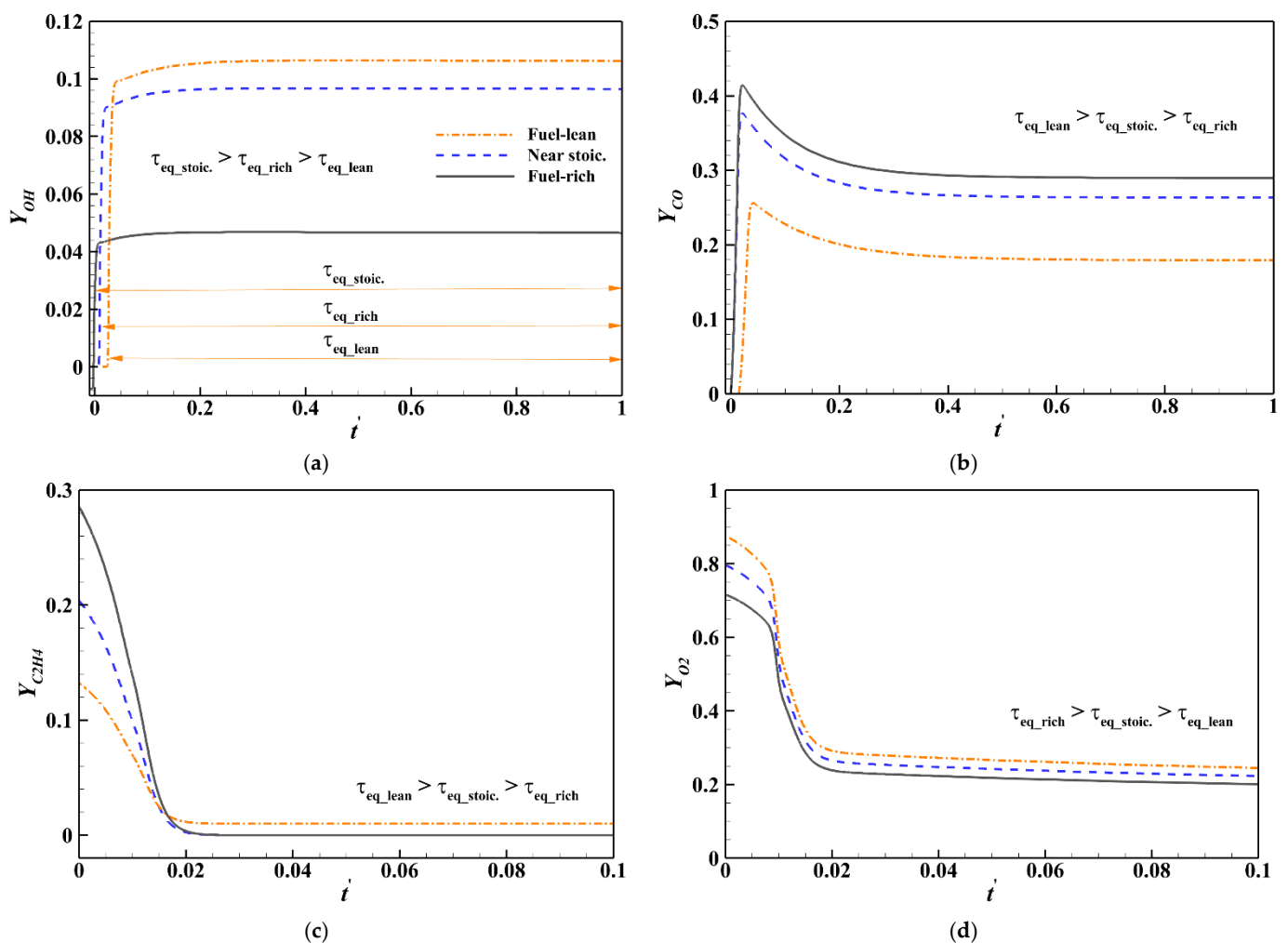


Figure 17. Variation in $\tau_{eq.}$ for (a) Y_{OH} , (b) Y_{CO} , (c) $Y_{C_2H_4}$, and (d) Y_{O_2} across different ϕ , ranging from lean to rich mixtures.

4. Conclusions

This study presents a 3D numerical analysis to investigate the characteristics of detonation waves in a non-premixed RDE fueled by C_2H_4 - O_2 across three equivalence ratio conditions: fuel-lean, stoichiometric, and fuel-rich. Simulations were conducted using a QG chemical mechanism and a discrete injection process. An extensive grid refinement

study was conducted to establish a baseline grid. Spatially, the detonation waves exhibit greater strength near the outer wall, transitioning into strong deflagrations near the inner wall. The radial difference in detonation structure is attributed to the C_2H_4/O_2 stratification resulting from incomplete mixing. On a macroscopic level, significant differences in detonation behavior are observed, influenced by variations in detonation height, the angle of the oblique shock, the vertical front, and back p . Notably, the high p region in the post-detonation zone expands as C_2H_4 levels increase. Regarding the structure of the detonation front, it has been observed that residual product gases from previous cycles remain within the chamber, potentially leading to incomplete combustion processes. The p contour along the outer wall reveals a less intense wave for the fuel-lean case. In the near-stoichiometric case, the outer-wall flow field exhibits a more intense and sharply defined gradient, signifying a more powerful and efficient detonation. The fuel-rich case shows signs of additional diffusion and mixing with a more dispersed wavefront likely due to the presence of unburned fuel. In contrast to the outer wall, the flow field observed at the mid-channel demonstrates a more stratified structure.

Numerical simulations reveal that discrete C_2H_4 injectors and slit-type O_2 injectors exhibit different stiffness characteristics, resulting in nonuniform fueling of the detonation chamber despite steady global flow rates when averaged over long periods. Critically, the injector recovery timescale adapts to the number of waves present in the chamber. To elucidate this further, instantaneous Y_s profiles on an axial–azimuthal slice are provided for three different mixtures. These profiles indicate that mixing predominantly occurs at a certain distance from the chamber inlet. Additionally, it is observed that the fuel stream impacts and flows along the outer wall. As the fuel flow rate increases, the mixing region expands downstream, and the impact of the fuel on the outer wall becomes more pronounced. The flow properties suggest that the reaction primarily takes place at the intersection of the fuel and oxygen streams and within the recirculation region. This dynamic interplay highlights the importance of injector design and placement in achieving efficient mixing and combustion in the detonation chamber. Cycle-averaged injection parameters indicate that the fuel injector exhibits stiffer dynamics compared to the oxidizer injector.

Characteristic chemical timescales are studied for fuel-lean, near-stoichiometric, and fuel-rich mixtures. The lean mixture, characterized by excess O_2 waves, exhibits less intensity and slower progression toward equilibrium and demonstrates prolonged reaction times. In contrast, the near-stoichiometric mixture exhibits superior performance metrics due to optimal fuel-oxidizer interactions. It achieves the most efficient combustion with the highest Θ , rapidly reaching equilibrium and exhibiting the shortest chemical reaction timescale. Across all conditions, highlighting its efficiency in sustaining robust detonation waves. The rich mixtures, with excess fuel, despite showing improved mixing compared to the lean case, also show a delayed approach to equilibrium and extended chemical reaction timescale. Across these mixtures, the induction timescale is generally 2–3 times longer than their respective chemical reaction timescale, while chemical equilibrium timescale spans a wide range of timescales, reflecting the complex, rapid dynamics inherent in these chemical processes. This study also highlights the significance of the characteristic chemical timescale in shaping the behavior of pre-detonation deflagration in RDEs. The results demonstrate that prolonged induction times under non-ideal equivalence ratios, combined with injector recovery dynamics, contribute to localized deflagration regions ahead of the detonation wave. Overall, this study significantly advances the understanding of RDE detonation physics, by addressing the intricate interplay of equivalence ratio, and injector behavior on detonation wave characteristics.

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resources, M.N.N.; data curation, M.N.N.; writing—original draft preparation, M.N.N.; writing—review and editing, M.N.N. and J.-Y.C.; visualization, M.N.N. and B.-K.S.; supervision, J.-Y.C.; project administration, J.-Y.C.; funding acquisition, J.-Y.C. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

p	pressure, atm
T	temperature, K
τ	timescale
t	cycle time
Y	mass fraction
Θ	thermicity, 1/s
u, v, w	velocity vectors, m/s
ρ	density, kg/m ³
e	total energy per unit volume, J/m ³
R	universal gas constant, J/kg.mol
M	molecular weight, kg/mol
h	enthalpy, J
c	specific heat capacity, J/kg·K
Δ	grid size
ϕ	equivalence ratio
U	velocity, m/s
ω	detonation wave speed, m/s
ns	nanosecond
μ s	microsecond
ms	millisecond

Subscripts

c	characteristics
$ind.$	induction time, s
$rxn.$	chemical reaction, s
$eq.$	chemical equilibrium, s
$res.$	chamber residence, s
$mix.$	reactant mixing, s
$avail.$	available mixing, s
$inj.rec.$	injector recovery, s
$inj.rev.$	injector flow reversal, s
$acoustic.$	acoustic, s
s	species
i	partial
0	chamber
VN	von Neumann
p	constant pressure, atm

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