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Impact of Fuel Injection Timing on Combustion Characteristics and Emissions in a Diesel Engine: A CFD Study

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Abstract:
This study employs combined 1D and 3D computational modeling to investigate the effects of fuel injection timing on combustion and emission performance in a diesel engine. Injections are timed at a baseline angle and further adjusted by +3, –3, and –6 crank angle degrees relative to baseline. Key parameters, including the in-cylinder pressure, temperature, heat-release rate, indicated work, and emission indices (NOx and soot), are compared across these cases. Results show that advancing injection timing consistently produces earlier ignition, higher peak pressure and temperature, and slightly higher indicated work and thermal efficiency, albeit with a marked increase in NOx. Conversely, retarding injection consistently lowers peak pressure and temperature, effectively reduces NOx formation, but leads to increased soot emissions and reduced efficiency. The CFD predictions leveraging an extended coherent flame model accurately replicate these observed effects. The findings highlight the inherent trade-offs in timing control: advancing injection can improve work output but aggravates NOx, while delaying injection reduces NOx at the cost of efficiency and a noticeable soot increase.

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1. Introduction

Modern diesel engines are central to heavy-duty applications due to their high thermal efficiency, multi-fuel adaptability, and durability [1, 2]. Consequently, they remain indispensable power sources for global transportation and industrial applications. However, increasingly stringent emissions regulations (e.g., Euro 7 and EPA Tier 4) necessitate advanced combustion control strategies to simultaneously reduce nitrogen oxides (NOx) and soot emissions, which exhibit a well-documented trade-off relationship [3]. These health concerns have forced engine designers to meet stringent emission regulations for NO_x and particulate matter without sacrificing efficiency [4].

In diesel combustion, precise control of injection parameters, including timing, is critical for optimizing performance and minimizing pollutants [4]. Fuel injection timing, in particular, is a primary control lever affecting ignition delay, combustion phasing, thermal efficiency, and emissions [5, 6]. The precise temporal coordination of fuel delivery relative to piston position determines the thermodynamic trajectory of the combustion event, thereby affecting both engine performance and pollutant formation mechanisms [7].

Fuel injection timing effects have been extensively studied in diesel engines through experiments and simulations. Research is well-established that injection timing controls ignition delay and premixed burn fraction [4, 5, 8, 9].

Advancing the timing (injecting earlier) initiates fuel delivery earlier during the compression stroke, generally increases ignition delay, and allows for more air–fuel mixing before ignition. This raises peak pressure and temperature during combustion [10]. Typically, this elevates peak cylinder pressure by better aligning combustion with top dead center, thereby increasing indicated work output and improving thermal efficiency [11, 12]. However, higher in-cylinder temperatures also promote NOx formation [5, 8]. For example, Baek et al. [4] report that advanced injection timing in a marine diesel engine raised the maximum combustion pressure and improved output (indicated work), consistent with increased premixed burn. Shuai et al. [5] similarly observed that advanced main injection reduced soot, CO, and hydrocarbon emissions (attributed to more complete fuel oxidation) but significantly increased NOx.

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Conversely, retarding injection shortens ignition delay and emphasizes diffusion-controlled combustion, which reduces NOx formation and peak temperatures and pressures [13]. However, this typically leads to increased CO2, total hydrocarbons, and soot due to incomplete mixing [9].

This fundamental trade-off between thermal efficiency and emissions was first quantified in seminal experimental work by Nehmer and Reitz [14], who demonstrated a 20% reduction in NOx emissions per 1 crank angle degree (CAD) retardation at the expense of 15% higher soot emissions. Subsequent research by Kook et al. [15] utilized high-speed imaging to reveal how advanced timing elongates liquid penetration length, increasing wall impingement risks that exacerbate unburned hydrocarbon emissions. Retarding injection reduces NOx and CO2 emissions (due to lower peak temperature), albeit with a modest rise in hydrocarbon emissions and slightly lower thermal efficiency. Ahmed et al. [9] warned that very early injection can cause fuel impingement and soot hotspots in wall-wetting scenarios. However, a delayed injection tends to lengthen the combustion duration and increase particulate emissions due to less complete mixing. Computational fluid dynamics (CFD) studies similarly reflect these behaviors [16, 17].

The literature also highlights practical limitations to timing variation. If the injection is too far advanced, combustion can occur too early, causing reverse torque and rough engine operation (as observed by Baek et al. [4]). As expressed in the previous paragraph, excessive advancing can even cause fuel impingement on the cylinder wall or piston, leading to incomplete burning and soot hotspots. For instance, Ahmed et al. [9] found that in a dual-fuel engine, using early injection timing along with high fuel oxygenation could optimize the efficiency-emission trade-off, but warned that very early injection risks wall-wetting of the spray. In summary, a controlled advance of injection timing is generally beneficial for efficiency, while retardation is used to cut NOx; choosing the exact timing requires balancing these effects.

CFD has emerged as an indispensable tool for deconstructing the multiphysics phenomena governing injection timing effects. The evolution of coupled 1D-3D simulation frameworks has enabled holistic analysis of gas exchange processes and combustion dynamics [18]. Critical to these advances has been the development of the extended coherent flame model (ECFM), which accurately captures turbulent combustion in stratified mixtures through a coherent flame surface density approach [19]. Mobasheri [16] validated ECFM-3Z-based CFD for timing effects. Further refinements incorporating detailed chemical kinetics, such as those by Pei et al. [20], have improved soot nucleation predictions through precise polycyclic aromatic hydrocarbon tracking.

Despite four decades of active investigation, key questions remain regarding isolated injection timing effects. A key challenge involves parametric confounding, where many studies concurrently modify multiple parameters (e.g., injection pressure, exhaust gas recirculation rates, or swirl ratios), obscuring causality in timing-specific responses [21]. Compounding this challenge are validation deficiencies, with limited research providing comprehensive CFD validation against spatially resolved soot-NOx measurements using advanced optical diagnostics, while most models rely on exhaust pipe emissions data and neglect in-cylinder stratification effects. Further complicating research is the neglect of cycle dynamics, where simulations predominantly assume steady-state conditions despite evidence of significant cycle-to-cycle variations, leaving transient effects during timing transitions poorly characterized. Underlying these issues is fundamental mechanistic ambiguity regarding whether soot reductions from advanced timing stem from improved oxidation [22] or suppressed formation pathways [23].

The prior findings set the stage for the present 1D-3D computational assessment. While the empirical soot-NOx trade-off is well-documented, this study provides novel, high-resolution CFD insights using an advanced turbulence model and dynamic meshing to capture in-cylinder processes accurately. Given the substantial impact of timing on both combustion phasing and emissions, this study performs a detailed CFD analysis of a diesel engine with an injection timing sweep. This isolates timing effects while holding chamber geometry and intake conditions constant. The goal is to quantify how small shifts in timing influence pressure-rise, heat release, indicated work, efficiency, and pollutant formation. The results will help engine designers choose the optimal timing setting that balances efficiency and emissions.

2. Methodology

A multi-stage simulation approach was employed. First, a one-dimensional engine model in AVL BOOST was calibrated to match key performance metrics. The engine specifications are shown in Table 1. Valve timing, intake/exhaust ducting, intercooler, and turbocharger maps were modelled so that the 1D model reproduced the experimentally measured in-cylinder pressure trace at the baseline timing case. From this 1D solution, the cylinder pressure and temperature history at intake valve closing timing are extracted to be used as initial conditions in the 3D combustion simulation.

Table 1. Engine Specifications

Parameter	Value
Engine Type	Water-cooled Turbo-Charged Heavy-Duty Diesel Engine
Number of Cylinders	12
Bore (mm)	150
Stroke (mm)	180
Engine Displacement (L)	38.1
Compression ratio (-)	15:1
Fuel Injection System	Common Rail Direct Injection
Rated Power (kW)	1000
Rated Speed (RPM)	1500

A moving mesh approach with crank-driven wall motion is implemented (dynamic mesh) to simulate the actual compression and expansion strokes with adaptive remeshing of the piston bowl region. The solver is AVL FIRE (an unstructured finite-volume CFD code). Dynamic meshing is performed in the FAME ENGINE Plus environment. The 3D mesh is a moving mesh with adaptive remeshing of the piston bowl region. Governing equations (mass, momentum, energy, and species) are solved with a turbulence model and a combustion model appropriate for diesel engine combustion modelling [16]. The three-equation k-ζ-f model is used for turbulence modelling in flow simulations. This model is widely applied in internal combustion engine flow simulations [24-29]. The Extended Coherent Flame Model (ECFM-3Z) is used to describe the coupling between turbulent flow and finite-rate chemistry in diesel combustion [16, 30]. This model tracks premixed, diffusion, and burnt zones and solves species transport for O2, CO, NOx, and soot precursors and has been widely applied in diesel engine CFD [16, 30]. The three-equation k-ζ-f model was developed by Hanjalić et al. in 2004 [31]. It is recommended for flows in complex domains where generating computational grids is challenging [32]. This model offers higher accuracy than the k-ε model and, unlike RSM or LES models, does not require extremely fine computational grids. A grid independence study was performed on the mesh template to ensure results were not sensitive to resolution. The chosen configuration provided a balance between computational expense and accuracy, with key outputs showing minimal variation (<5%) compared to a finer reference mesh. The FAME ENGINE Plus environment maintained mesh quality throughout the simulation.

Fuel injection is modelled by specifying the nozzle geometry and injection profile corresponding to the engine's single-point injector. The injection timing is varied relative to baseline as follows: 3 CAD advance, base timing, 3 CAD retard, and 6 CAD retard. The injection timing sweep is selected to be representative of the practical calibration range for diesel engines, capturing the transition from premixed-dominated to diffusion-dominated combustion and its associated impact on the performance and emissions trade-off. All other parameters are held fixed, including the intake air (100% dry air, fixed charge temperature and pressure) and combustion chamber geometry. The spray model includes sub-models for spray-wall interaction. The dynamic mesh capabilities of the FAME ENGINE Plus environment were used to ~~accurately~~ capture piston motion and geometry deformation accurately, ensuring correct spray targeting. Analysis confirmed that significant liquid wall film formation did not occur for the injection timings investigated. For each case, the simulation is run through one engine cycle to reach steady cyclic operation, and the in-cylinder pressure, heat release, species fields, and flow variables are recorded. Post-processing computes indicated work and thermal efficiency from the pressure trace, and NOx and soot emissions from the chemical reaction model outputs. This methodology aligns with established practice in diesel engine CFD [12, 17]. For example, Baek et al. [4] used in-cylinder pressure diagnostics to adjust timing on a marine engine.

Figure 1 and Table 2 demonstrate strong agreement between experimental data and the coupled 1D/3D simulation for pressure, NOx, and soot emissions, respectively. The predicted in-cylinder pressure curve (Figure 1) matches the experimental peak within 3%, while NO_x and soot emissions (Table 2) fall within a ±3% margin. These results are consistent with similar CFD validation studies—such as the study by Husberg et al. [33], who reported tight alignment between experimental pressure, NOx, and soot traces using advanced CFD, and the integrated 1D–3D framework for NOx and soot predictions. These results validate the robustness of the applied model in capturing pressure dynamics and trends in emission formation under varying injection timings. Model validation ensured reliability (3% deviation) before executing timing sensitivity runs. By using the validated models, the present study ensures that timing is the only variable, while geometry and intake conditions are held constant, allowing the observed changes in pressure, temperature, and emissions to be attributed solely to the timing shifts. Validation was performed against experimental in-cylinder pressure and global emission data. Spatially resolved validation data (e.g., for equivalence ratio or temperature) were not available for this engine setup but remain an area for future work. The advanced turbulence modelling (k-ζ-f) provides increased confidence in the predicted in-cylinder processes.

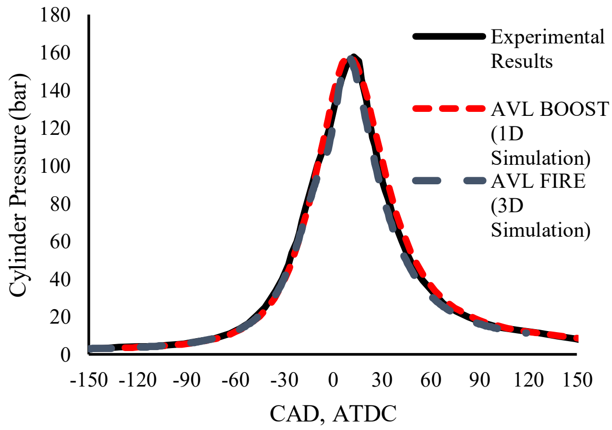

Figure 1. **Comparison between experimental and numerical (1D/3D) modeling results of engine cylinder pressures**

Table 2. **Experimental vs. 3D simulated NOx and soot emissions comparison in the engine**

Parameter	Experimental (ppm)	3D Simulation (ppm)	Relative Error (%)
Soot	12.35	12.40	+0.40%
NOx	4122.00	4008.00	−2.77%

3. Results and Discussion

Figures 2 and 3 show the simulated cylinder pressure and mean temperature traces through the engine cycle for the four injection timing cases. Advancing the injection by 3 CAD causes the start of combustion to occur earlier (the ignition delay is effectively shortened), so the pressure rise and heat release happen when the piston is still closer to the

TDC. As a result, the maximum cylinder pressure and temperature are higher in the advanced timing case than in the baseline. Conversely, retarding the injection (by 3 or 6 CAD) means fuel is injected later in the cycle, where the piston is already descending. Hence, the peak occurs at a lower compression and temperature. The peak cylinder pressure and temperature are thus lower for the delayed cases compared to the base. This behavior is expected: when fuel is injected earlier, more time is available for the premixed burn and more work is done during the compression stroke, raising the peak pressure. Quantitatively, the CFD predicts a roughly 3% increase in maximum pressure for a 3 CAD advance and a corresponding decrease for a 6 CAD delay.

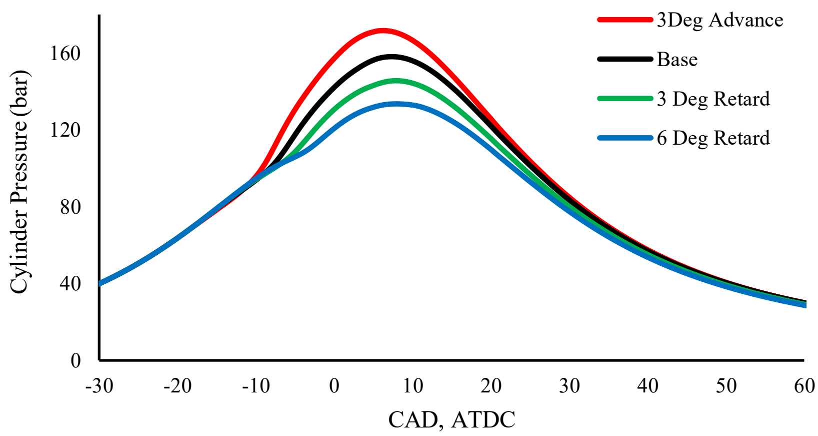

Figure 2. **In-cylinder pressure profiles versus crank angle degree under different fuel injection timing conditions**

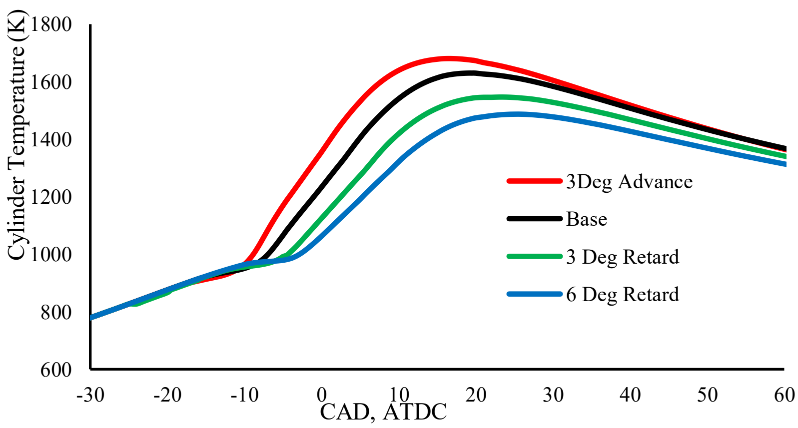

Figure 3. **Mean in-cylinder temperature profiles versus crank angle under different fuel injection timing conditions.**

The temperature distributions (not just mean temperature) also reflect this trend. In the advanced case, higher local temperatures develop earlier (see Figure 4) at TDC, confirming that combustion is more intense. Delaying the injection suppresses the peak temperature. These peak pressure and temperature shifts have direct consequences for work output and emissions, as discussed below.

The rate of heat release as a function of crank angle is plotted in Figure 5. Advancing injection timing shifts the entire heat release curve earlier in the cycle. As noted above, earlier injection leads to an earlier ignition; thus, the main heat release starts sooner and reaches its peak earlier when the cylinder pressure and temperature are rising. This results in a slightly higher peak heat release rate as well (due to higher pressure and temperature). The area under the heat release rate curve (total heat released) is essentially the same (same fuel mass), but its timing is advanced. In contrast, delaying the injection postpones ignition, so the heat release ramp-up occurs later (the curve is shifted to the right) and its peak magnitude is slightly reduced because the peak pressure/temperature is lower. In other words, advanced timing yields a quicker and more vigorous burn, while retarded timing produces a slower burn.

Figures 6 and 7 provide additional insight. At TDC, the equivalence ratio is higher near the injector region for the advanced injection case, indicating a richer premixed charge by TDC. Meanwhile, turbulence kinetic energy is also higher for advanced timing (Figure 7), because the fuel spray has longer to mix and generate turbulence before TDC. This increased turbulence can enhance the flame propagation post-ignition, further increasing the burn rate.

The integrated pressure crank angle curve gives the indicated work. Figures 8 and 9 compare the indicated work and thermal efficiency under each timing. As expected, the advanced injection case produces the highest indicated work and slightly higher indicated thermal efficiency. With combustion starting earlier and at a higher pressure, more of the heat release occurs while the piston is still moving upward, effectively converting combustion energy into work. In contrast, the delayed injection cases yield less indicated work and lower efficiency. Delaying the injection means that more of the heat release occurs as the piston descends (resulting in less useful work) and more heat is lost to the walls and exhaust. Specifically, the 6 CAD delayed case shows the most significant drop in work and efficiency (compared to the base), whereas the 3 CAD advanced case shows a modest gain. These trends are consistent with the pressure profiles. Higher pressure in the advanced case yields higher work, while the lower pressure in the delayed case reduces work.

Quantitatively, the CFD predicts about a 2–3% increase in indicated thermal efficiency for the 3 CAD advance case, and about a 11–12% decrease for the 6 CAD delay case, relative to base. These efficiency shifts are modest but significant for engine performance.

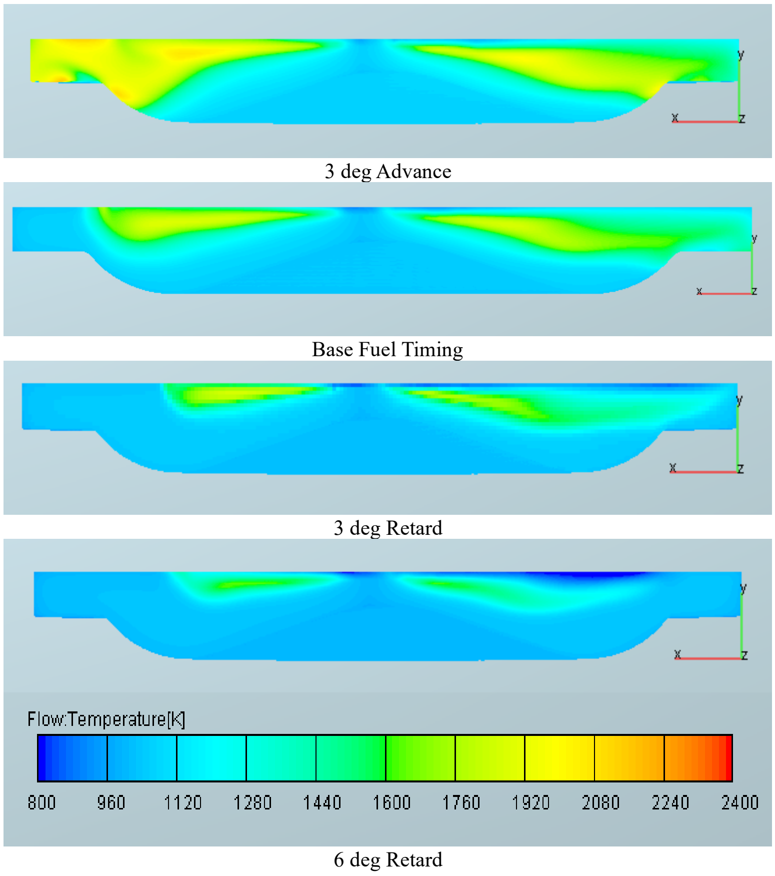

Figure 4. **Temperature distribution under different fuel injection conditions at top dead center**

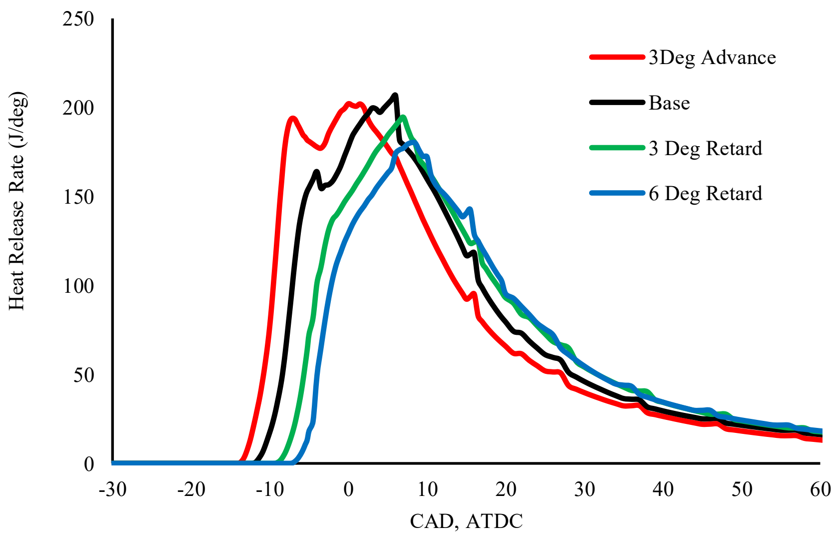

Figure 5. **Heat release rate profiles versus crank angle under different fuel injection timing conditions**

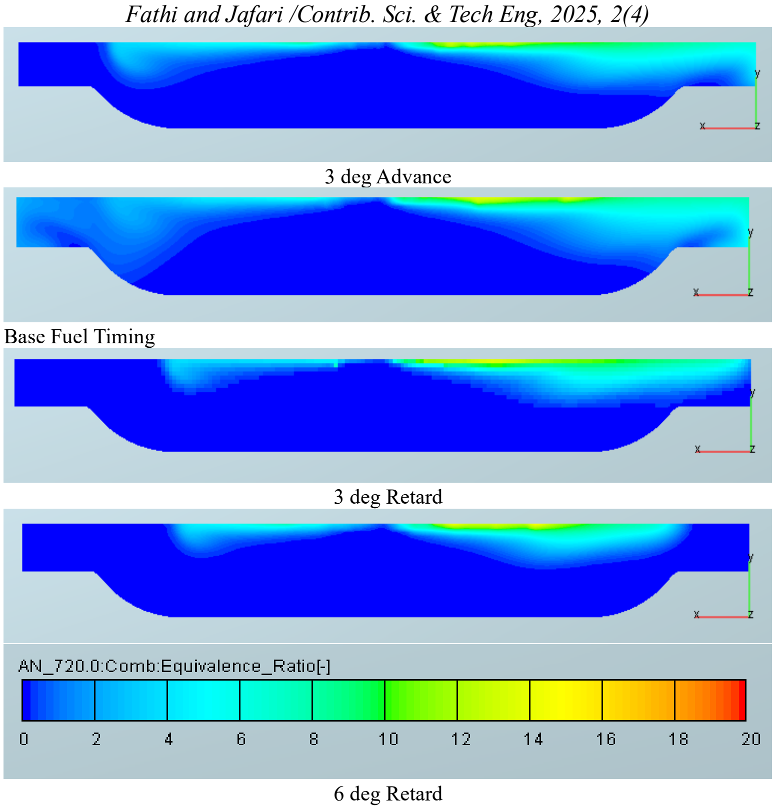

Figure 6. **Equivalence ratio distribution under different fuel injection conditions at top dead center**

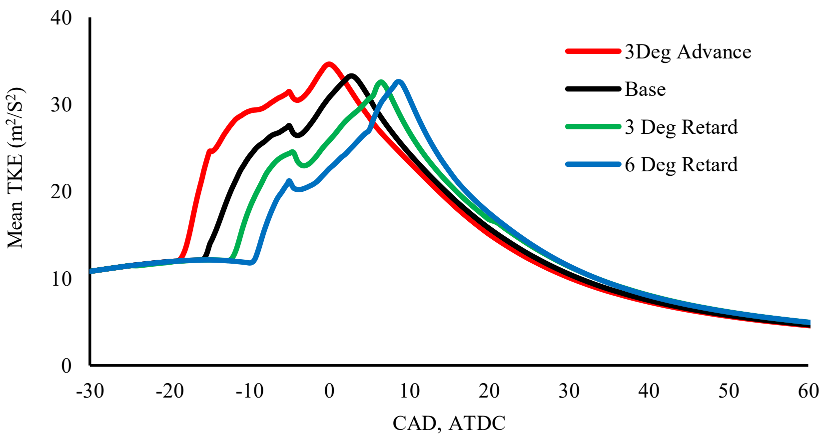

Figure 7. **Mean turbulence kinetic energy (TKE) profiles versus crank angle under different fuel injection timing conditions**

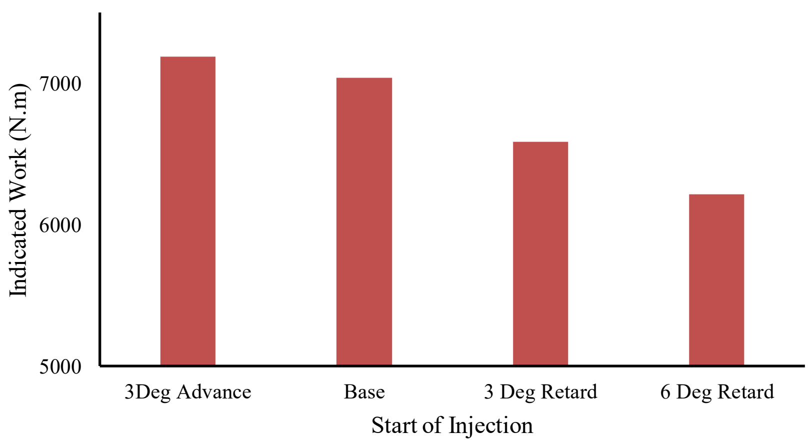

Figure 8. **Indicated work output under different fuel injection timing conditions**

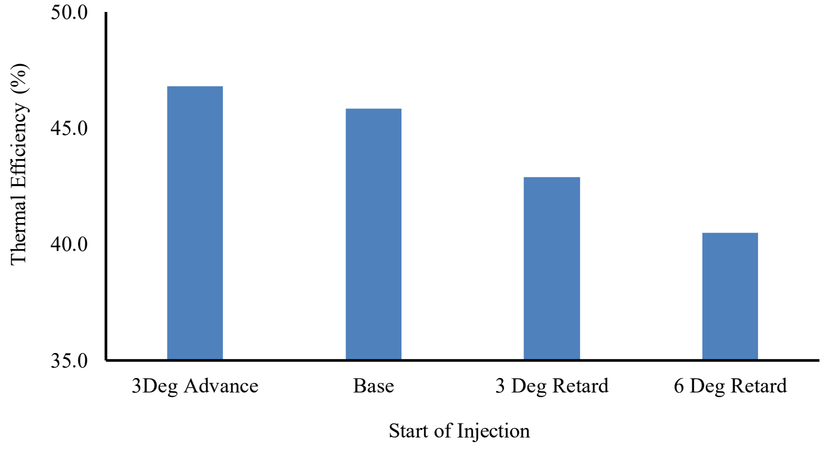

Figure 9. **Indicated thermal efficiency under different fuel injection timing conditions**

Figures 10 and 11 summarize the key emission results. As shown in Figure 10, NOx emissions increase markedly with advanced injection timing and decrease with retarded injection. This inverse trend with soot (discussed next) is expected: earlier injection raises the peak cylinder temperature and pressure (providing more thermal NOx formation time and available oxygen). In contrast, delaying the injection lowers the peak temperature, thus suppressing NOx. Quantitatively, the 3 CAD advance case produces the highest NOx, while the 6 CAD delay case shows the lowest NOx.

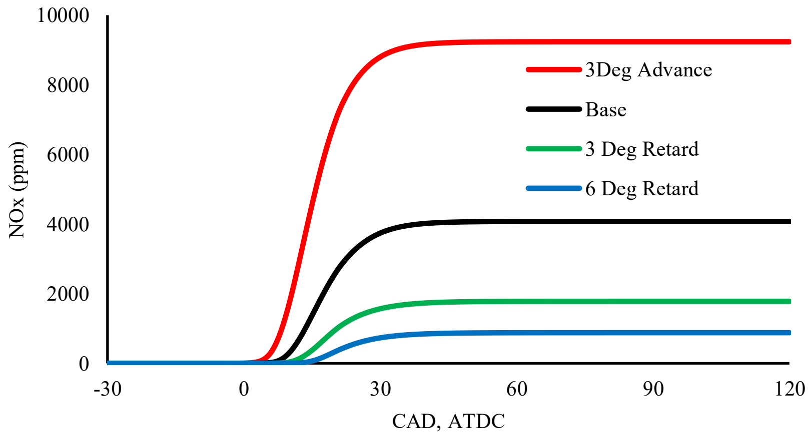

Figure 10. **NOx emissions profiles versus crank angle under different fuel injection timing conditions**

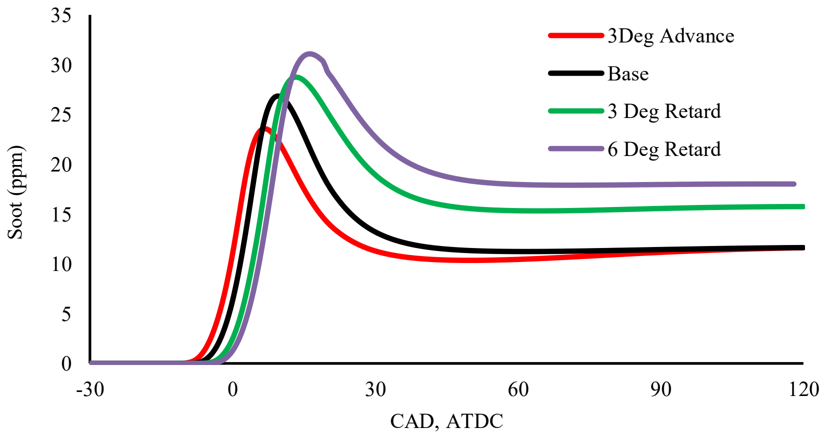

Figure 11. **Soot emissions profiles versus crank angle under different fuel injection timing conditions**

Meanwhile, soot emissions (particulate matter) show the opposite trend. In Figure 11, the advanced injection case has somewhat the lowest soot, and the delayed case has the highest soot. This occurs because advanced timing promotes more complete combustion in the high-temperature region (less diffusion soot). By injecting earlier, the fuel has more time to mix with air before the onset of ignition, reducing fuel-rich pockets that produce soot. Delaying injection, however, means more fuel is injected into a denser, colder environment (piston descending), which tends to form larger soot particles and higher overall particulate yield.

These results align with the classical NOx–soot trade-off. Advanced timing improves mixing and reduces soot to some extent, but it sharply increases thermal NOx. Conversely, delayed timing suppresses NOx at the expense of higher soot. They are consistent with previous reports. Shuai et al. [5] found that advanced injection lowered soot while raising NOx. In this engine, retarding timing is an effective NOx control measure (reducing NOx by ~70–80% in the 6 CAD case), while increasing soot by about 50%.

In summary, the CFD results clearly demonstrate that injection timing must be carefully chosen to balance efficiency and emissions. In the baseline geometry and load, the 3 CAD advanced case gave the best power output, but at a significant NOx cost. In comparison, the 6 CAD delay case minimized NOx significantly but degraded efficiency. An intermediate compromise (perhaps a slight advance or base timing) might be optimal depending on which pollutant is targeted. These findings quantitatively illustrate the qualitative engine behavior noted in the literature by Ahmed et al. [9]. Table 3 provides normalized performance indicators for injection timing shifts, guiding engine calibration decisions. Therefore, recommendations for engine designers can be summarized as follows:

- 3 CAD Advance: For performance-oriented settings, enabling maximum efficiency and acceptable soot, but with highly increased NOx output.
- Baseline: Offers balanced performance with moderate emissions.
- 3 CAD Retard: Suitable when NOx reduction (~60%) is desired with minimal efficiency loss.
- 6 CAD Retard: Best for stringent NOx control, though with significant trade-offs in efficiency and increased soot.

Table 3. Normalized performance indicators for injection timing shifts

Timing Shift (CAD)	Thermal Efficiency (%)	NO_x Change (%)	Soot Change (%)
+3	+2.2	+126.6	0
0	—	—	—
–3	–6.3	–56.3	+33.3
–6	–11.6	–78.4	+50

4. Conclusion

This CFD study of a diesel engine confirms that fuel injection timing has a pronounced impact on combustion and emissions when geometry and intake are held fixed. Advancing the timing (by 3 CAD in this case) raises the in-cylinder peak pressure and temperature, accelerates heat release, and slightly improves indicated work and efficiency. However, this comes with a sharp increase in NOx formation. Conversely, retarding injection (3 or 6 CAD late) lowers peak pressure and temperature, reduces NOx, but increases soot and reduces output. The computed trends mirror classical diesel behaviour and align with previous experimental and simulation studies.

Specifically, the +3 CAD timing case showed the highest pressure, work, and NOx, whereas the –6 CAD case showed the lowest pressure, the lowest NOx, but the highest soot. The trade-offs observed here highlight the need for careful timing optimization. The optimal timing, therefore, depends on the priority, such as emission standards or fuel economy targets. If the goal is maximum efficiency or power, a moderately advanced timing (relative to stock setting) often yields the best balance in modern engines (at the expense of emission levels); if NOx control is paramount, a slight delay is beneficial (at the expense of efficiency and soot). The CFD results were found to be reliable by comparison to known patterns.

This study established a baseline understanding of the injection timing trade-off using fixed intake conditions. The critical interaction between injection timing and exhaust gas recirculation is a logical and essential next step. In practice, combining timing adjustments with other controls (e.g., exhaust gas recirculation, multiple injections, and water injection) would be necessary to meet strict emissions standards; however, this study provides a clear isolation of the timing effect. Future work will build upon this validated baseline model to explore how the optimal timing window shifts under conditions representative of real-world engine calibration.

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