

Transient Build-up and Effectiveness of Diesel Exhaust Gas Recirculation

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ABSTRACT

Modern diesel engines employ a multitude of strategies for oxides of nitrogen (NO_x) emission abatement, with exhaust gas recirculation (EGR) being one of the most effective technique. The need for a precise control on the intake charge dilution (as a result of EGR) is paramount since small fluctuations in the intake charge dilution at high EGR rates may cause larger than acceptable spikes in NO_x/soot emissions or deterioration in the combustion efficiency, especially at low to mid-engine loads. The control problem becomes more pronounced during transient engine operation; currently the trend is to momentarily close the EGR valve during tip-in or tip-out events. Therefore, there is a need to understand the transient EGR behaviour and its impact on the intake charge development especially under unstable combustion regimes such as low temperature combustion.

This study describes a zero-dimensional EGR model that enables the estimation of transient (cycle-by-cycle) build-up of EGR and the time (engine cycles) required to reach steady-state EGR operation (intake/exhaust concentrations). The model response is tuned to a multi-cylinder engine by using an overall engine system time-constant. The effect of EGR on the cylinder charge has been examined in terms of the intake charge dilution and the excess-air ratio. The intake dilution has been empirically shown to provide a reliable quantitative measure of the EGR effectiveness in reducing NO_x emissions. The EGR analysis is validated against a wide range of engine operations.

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INTRODUCTION

Modern diesel engines achieve low oxides of nitrogen (NO_x) emissions through a multitude of in-cylinder combustion modifications as well as exhaust aftertreatment devices. Among the various in-cylinder techniques such as injection timing retard, exhaust gas recirculation (EGR), intake boost, injection rate shaping etc., EGR is the principal method used in modern diesel engines for reducing NO_x emissions [1, 2, 3]. However, the use of EGR generally results in higher particulate matter (PM) production [4,5]. To overcome the resulting NO_x-PM trade-off, physical improvements in the air and fuel systems (multi-stage turbocharging, common rail injection systems, variable valve timing etc.) as well as alternate combustion regimes that reduce the combustion temperatures and improve the homogeneity (mixing) of the cylinder charge, are being actively pursued [1,6,7]. The reduced temperatures inhibit the NO_x production while the enhanced mixing reduces the propensity for soot formation by avoiding localized stoichiometric/rich burning, so that ultra-low levels of NO_x and PM can be concurrently achieved.

The common strategies for achieving low temperature combustion (LTC) include homogenous charge compression ignition (HCCI) [8, 9, 10], smokeless rich combustion (also called modulated kinetics combustion) [11, 12, 13], and reactivity controlled compression ignition (RCCI) [14, 15, 16] as shown in Figure 1.

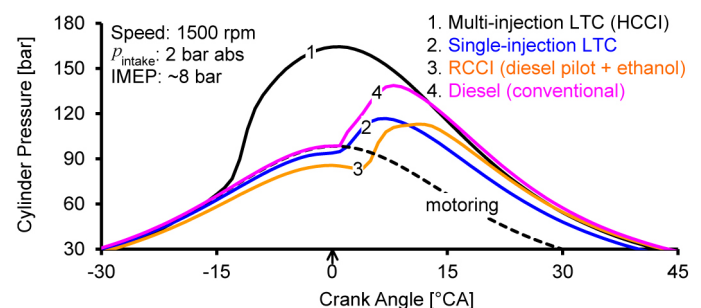


Figure 1. Advanced Combustion Modes for Diesel Engines [16]

HCCI combustion is characterized by earlier than top-dead-centre (pre-TDC) phasing, very high pressure rise rates, short combustion durations, and minimal control over the timing of the combustion event. To offset the high reactivity of the diesel fuel, large amounts of EGR (30 to 60%) are usually applied to postpone the initiation of combustion, shift the combustion towards TDC and alleviate to some extent, the high pressure rise rates and the reduced energy efficiency. However, as the fuelling and the engine load increases, the diesel HCCI combustion is severely limited by the physical constraints of the engine [8, 9, 10].

The single-injection LTC, on the other hand, relies on large amounts of EGR (typically 50~70%) to withhold the air-fuel mixture from combustion [13]. The highly-diluted cylinder charge (8~12% intake oxygen) makes the combustion sensitive to small changes in EGR - a slight increase in EGR (1~2%) can rapidly deteriorate the combustion stability, often resulting in mis-fire; conversely, a sharp increase in the soot emissions can occur for a small drop in the EGR rate. The single-injection LTC, thus materializes close to the limiting conditions, requiring a tighter control on the operating conditions compared to the conventional diesel high temperature combustion (HTC). The engine load level of the single-injection LTC is limited to low loads/low engine speeds [13] because the ability to separate the fuel injection from the combustion event diminishes rapidly with increased fuelling rate.

The major challenges of LTC strategies such as HCCI can be overcome with dual-fuel RCCI combustion in which the reactivity of the cylinder charge is modified by using a highly reactive fuel (pilot injection) to ignite the bulk low reactivity fuel (main contributor to power production) under lean, EGR diluted conditions [14, 15, 16, 17, 18]. Previous results indicate that moderate to high engine loads are achievable with RCCI combustion while retaining or exceeding diesel-like thermal efficiencies. Moreover, the lean premixed nature of the bulk phase of combustion ensures that low to moderate EGR levels are sufficient to maintain NO_x to ultra-low levels while soot emissions are practically close to zero.

While all these modes of combustion target the minimization of NO_x and soot production, they are uniquely different in terms of the operability limits and combustion characteristics (Figure 1), with significantly wide-ranging EGR requirements [9,16,19]. For practical implementation of these combustion modes, mode-switching needs to be carried out on-the-fly, with the ability to adapt the air, EGR and the fuel systems within a few engine cycles to the new mode [20,21] as shown in Figure 2. This requires the EGR quantities to be tracked and estimated precisely during the transition cycles, which is impeded by the lack of robust feedback on the amount of recycled gases. The problem is compounded by the disproportionate response times of the air-path system and the combustion system. The current trend in production vehicles is to shut off EGR during transients since the EGR valve opening for steady-state operation is mostly based on look-up tables calibrated during the development stage, with a few model-based corrections.

Therefore, there is a need to track the EGR quantity and the resulting intake charge dilution during transient load and intake pressure changes so as to enable the use of EGR.

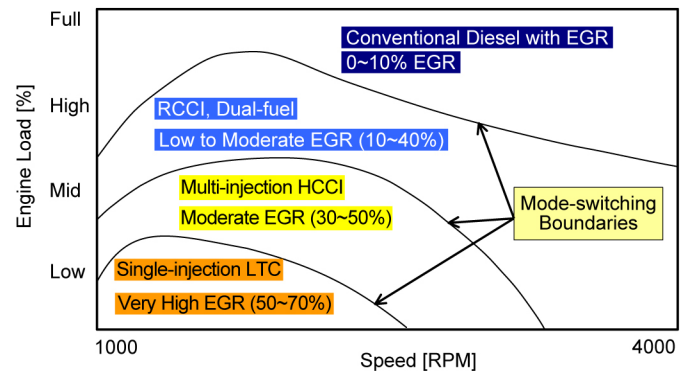


Figure 2. Mode-switching Requirements for LTC Implementation

While these LTC strategies look promising, the difficulties in the implementation of these advanced combustion modes at the production level, have resulted in exhaust aftertreatment devices such as selective catalytic reduction (SCR) to be widely used to meet the legislative NO_x requirements. However, even with the LNT or SCR-urea approach, the raw engine-out NO_x has to be reduced to 50~200 ppm for efficient operation of these devices. This is primarily achieved by using moderate to large amounts of EGR.

There has been extensive research, both theoretical and empirical, on the fundamental impacts of EGR on diesel combustion and emissions under steady-state engine operation [1, 2, 3, 22, 23, 24, 25, 26, 27]. Zheng et al. [1] outlined the requirements and limitations for the physical implementation of EGR on diesel engines using high-pressure loop and low-pressure loop systems. They also proposed treatment of the EGR stream (cooling, oxidation, fuel reforming) to deal with the combustion instabilities as a result of EGR application and also highlighted the need for real-time EGR feedback for enabling transient EGR operation. Zhao et al. [22] developed an engine simulation model with detailed chemical kinetics to analyse the effects of the recycled gases on HCCI combustion. Aithal [23] reported the development of a 0-D modelling tool to quantify the impact of EGR on diesel combustion parameters under steady-state conditions. There is extensive literature available on the development of multi-zone engine cycle simulations models [24, 25, 26, 27]. Benson and Whitehouse provided a comprehensive description of the combustion, heat transfer and NO_x emission sub-models as well as a step-by-step guide to setup zero-dimensional simulations [24]. Rakopoulos et al. [25] included spray development, air entrainment and soot emission sub-models in their two-zone models. Sahin and Durgun [26] also presented a multi-zone diesel model for estimating performance and emission metrics but did not account for the in-cylinder residual gases or EGR. Xue and Caton [27] demonstrated a 6-zone model for diesel combustion based on Dec's conceptual spray jet model. Although they included the effects of EGR, they

not account for the in-cylinder residuals and the model only dealt with stabilized, steady state operation.

In this work, the development of a zero-dimensional EGR model has been described in detail, including a step-by-step guide for interfacing the EGR sub-model to any existing engine-cycle simulation code. The sub-model can be used for both transient and steady-state engine simulations and enables the estimation of cycle-by-cycle build-up of EGR and the time (engine cycles) required to reach steady-state EGR operation (intake/exhaust concentrations). A simplified approach is adapted for tuning the model to a multi-cylinder engine by using an overall engine system time constant that provides adequate performance matching over the engine operating map. The effect of EGR on the cylinder charge has been examined in terms of the intake charge dilution. The transient and steady-state EGR estimations are validated against a wide range of engine operations.

EGR MODEL DEVELOPMENT

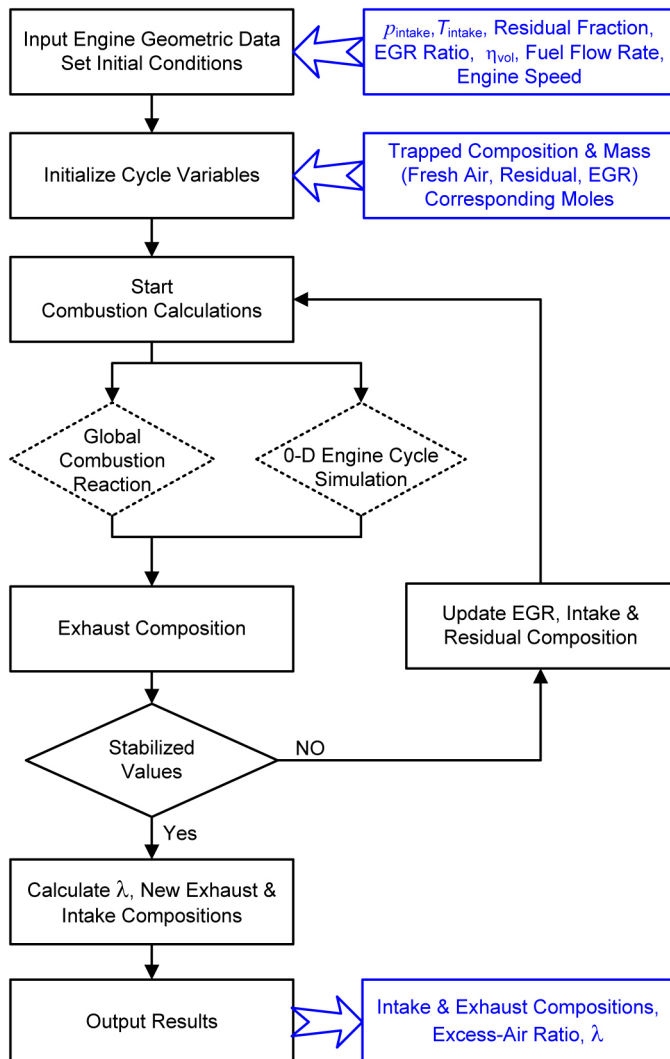


Figure 3. Flow Chart of EGR Calculation Algorithm

A zero-dimensional EGR model was developed so that the intake and exhaust concentrations could be calculated on a mass basis. The residual mass fraction was also included so that the effect of increased residuals with higher exhaust backpressure could be analysed.

The flowchart for implementation of a zero-dimensional EGR simulation is shown in Figure 3. The model can either be integrated with a zero-dimensional engine cycle simulation or a global combustion reaction can be employed for a quicker assessment of the EGR. The analysis only considers the complete products of combustion for a lean-burn engine, i.e. carbon dioxide, water, nitrogen and oxygen. The assumptions for the calculation are as follows:

- The moles of the in-cylinder charge, M_{cyl} are fixed and calculated based on the initial conditions that include the intake pressure/temperature and engine geometric constraints.
- The EGR stream is assumed to be fully cooled and at the same temperature as the fresh air part of the intake charge, i.e. $T_{egr} = T_{int}$.
- The EGR ratio is taken as the mass fraction of the exhaust. Therefore, the quantity of the recycled gases is calculated by multiplying the EGR ratio with the mass of the exhaust (mass of intake charge + mass of injected fuel).

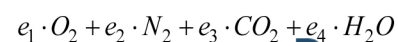
$$r_{egr} = \frac{\dot{m}_{egr}}{\dot{m}_{air} + \dot{m}_f + \dot{m}_{egr}} \quad (1)$$

- For the residuals, the composition will be the same as that of the exhaust. The residual fraction depends on the volumetric efficiency η_{vol} , the engine speed and the exhaust back-pressure. If the dynamics of the intake & exhaust processes are accounted for in the engine cycle simulation, then the model will compute the residual fraction r_{res} . In case of a closed cycle simulation only, the residual fraction r_{res} needs to be assigned so that

$$r_{res} = 1 - \frac{m_{int}}{m_{cyl}} \approx 1 - \eta_{vol}$$

- The compositions of the intake and residual portions of the cylinder charge are updated at each iteration until a stable exhaust composition is attained (model stabilization criterion of 0.2% relative change in the calculated exhaust oxygen concentration from cycle-to-cycle after the application of EGR was used in this work).
- The excess-air ratio is obtained by first calculating the air/fuel ratio on a mass basis and then dividing with the mass-based stoichiometric air/fuel ratio for the diesel fuel.

At the end of $(k-1)^{th}$ engine cycle, the species in the exhaust are as follows:



The total moles of exhaust will be:

$$M_{exh} = \sum_{i=1}^4 e_i$$

where $i = \{O_2, N_2, CO_2, H_2O\}$.

The molecular weight and the mass of exhaust can then be calculated as follows:

$$MW_{exh} = \sum_{i=1}^4 \left(\frac{e_i}{M_{exh}} \cdot MW_i \right)$$

$$m_{exh} = M_{exh} \cdot MW_{exh} \quad (3)$$

If EGR is now applied at a rate of r_{egr} , the corresponding EGR attributes are as follows:

$$m_{egr} = m_{exh} \cdot r_{egr}$$

$$M_{egr} = \frac{m_{egr}}{MW_{exh}} \quad (4)$$

The corresponding moles of species in EGR will be:

$$b_1 \cdot O_2 + b_2 \cdot N_2 + b_3 \cdot CO_2 + b_4 \cdot H_2O \quad (5)$$

where

$$b_i = M_{egr} \cdot \frac{e_i}{M_{exh}} \quad (6)$$

For the residuals,

$$m_{res} = r_{res} \cdot m_{cyl}$$

$$M_{res} = \frac{m_{res}}{MW_{exh}}$$

The residual composition is:

$$r_1 \cdot O_2 + r_2 \cdot N_2 + r_3 \cdot CO_2 + r_4 \cdot H_2O \quad (7)$$

where

$$r_i = M_{res} \cdot \frac{e_i}{M_{exh}} \quad (8)$$

For the k^{th} engine cycle, the total moles of the intake charge will be:

$$M_{int} = M_{air} + M_{egr}$$

where $M_{int} = M_{cyl} - M_{res}$. The total mass of the intake charge therefore becomes equal to:

$$\dot{m}_{int} = \dot{m}_{air} + \dot{m}_{EGR} \quad (9)$$

The fresh air part of the intake will be:

$$M_{air} = M_{int} - M_{egr} \quad (10)$$

The mass of fresh air will be:

$$m_{air} = M_{air} \cdot MW_{air} \quad (11)$$

where the molecular weight of fresh air is assumed constant and equal to 28.84 kg/kmol (based on simplified air composition: 20.95% O_2 , balance Nitrogen).

The corresponding moles of species for the fresh air are:

$$a_1 \cdot O_2 + a_2 \cdot N_2 + a_3 \cdot CO_2 + a_4 \cdot H_2O \quad (12)$$

where

$$a_1 = M_{air} \cdot 0.2095$$

$$a_2 = M_{air} \cdot 0.7905$$

$$a_3 = a_4 = 0$$

The total intake composition then becomes:

$$n_1 \cdot O_2 + n_2 \cdot N_2 + n_3 \cdot CO_2 + n_4 \cdot H_2O \quad (13)$$

where

$$n_i = a_i + b_i \quad (14)$$

The intake composition will be the input to the closed-cycle part of the zero-dimensional simulation for the k^{th} cycle. The process will be repeated as per Figure 3 until the calculated intake/exhaust compositions converge to stabilized values.

Global Combustion Reaction

A quick and fairly accurate approximation of the EGR can be achieved using a global combustion reaction (without dissociation). The active constituents participating in the