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Effect of Exhaust Gas Recirculation in NOx Control for Compression Ignition and Homogeneous Charge Compression Ignition Engines

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Abstract

Exhaust Gas Recirculation (EGR) is a potential option for controlling in-cylinder NOx in automobiles. This paper aims to study the effect of EGR on NOx emissions and in Compression Ignition (CI) engines at various conditions. To this end, low dimensional models are developed using a first principles approach without recourse to empirics. Fuel oxidation represented by a three-step global kinetic model coupled with the Zeldovich mechanism for NOx formation is used to predict the composition of the entire spectrum of engine-out gases. Solution of the conservation equations using MATLAB provides the in-cylinder variation of parameters like volume, pressure, torque, speed and work done and species (Fuel, CO, CO_2, NO_X, etc.) with respect to Crank Angle Displacement (CAD). The inlet conditions are the fuel-air equivalence ratio, engine specifications and the inlet air temperature. The simulations are validated against experimental pressure profiles from the literature. External EGR is then implemented to study its effect on engine-out emissions under cold start conditions. The effect of EGR at various combinations of engine operating conditions is examined in detail.

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1. Introduction

Internal Combustion (IC) engines that are cyclic devices have the ability to convert chemical energy of fuel into mechanical energy by combustion of the fuel. In contrast to the SI Engine, air is compressed to high pressures by the piston movement in a CI engine, over which fuel is sprayed; and the fuel auto-ignites due to the compression. Homogeneous Charge Compression Ignition (HCCI) engine offers the advantages of both the CI and SI engines. It runs on a pre-mixed Air-fuel mixture and produces lower NOx similar to SI engines and ignites via compression, and without the need for a spark, like CI engines.

The engine-out emissions pose deleterious effects on the environment and composition of earth's atmosphere. Considering the effects of exhausts from IC engines on the environment, and the increase in the number of automobiles plying on the road, different countries have come up with stringent legislation

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to regulate the harmful engine-out emissions. Emission norms and the need for control of pollutants in the environment drive the need for efficient and cost-effective engine design and emission treatment systems. Hence, it has become imperative that we understand the combustion phenomenon in IC engines in considerable detail.

In this work, an engine model is derived from basic principles of conservation of various quantities, with reasonable assumptions, in order to predict engine performance in terms of various operating parameters. The emission control methods used or proposed currently include after-treatment devices and in-cylinder modifications. Here, the in-cylinder modification, Exhaust Gas Recirculation (EGR), is analysed.

This work focuses on developing a low dimensional kinetics-based model for diesel engine combustion. Unlike the models in literature, which are based on thermodynamics, experimental data or on average calorific values [1], this model uses kinetic expressions to capture the heat released by combustion. EGR is then implemented and the effect of %EGR on NOx is studied. HCCI simulations were carried out using the commercial package DARS in order to compare the effects of EGR in NOx control in the two kinds of engines.

2. Modeling of HCCI Engines

A zero dimensional stochastic model is used for modelling the HCCI engine in the commercial package DARS. The Stochastic model is conceived as a probability density function (PDF) consisting of a discrete number of particles. The number of particles is a measure of the accuracy and computational load. The transient MDF is assumed to be a partially stirred tank reactor with the following equation containing the flow, source and mixing terms [2]:

$$\frac{\partial}{\partial t}F_\phi(\psi,t)=\frac{\partial}{\partial\psi_{S+1}}\left(V\frac{1}{Cp}\frac{dp}{dt_{\Delta V}}F_\phi(\psi,t)\right)+\frac{C_\phi\beta}{\tau}\left[\int_{\Delta\phi}F_\phi(\psi-\Delta\psi,t)F_\phi(\psi+\Delta\psi,t)-F_\phi(\psi,t)\right]+$$
$$\frac{\partial}{\partial\psi_{S+1}}\left(V\frac{1}{Cp}\frac{dp}{dt_{mix}}F_\phi(\psi,t)\right)-\left(\frac{\partial}{\partial\psi_{S+1}}\left(\frac{1}{Cp}\sum_{i=1}^{S}h_i\frac{M_i}{\rho}\omega(\phi)F_\phi(\psi,t)\right)-\sum_{i=1}^{S}\frac{\partial}{\partial\psi_i}\left(\frac{M_i}{\rho}\omega(\phi)F_\phi(\psi,t)\right)\right)+$$
$$\frac{\partial}{\partial\psi_{S+1}}\left(V\frac{1}{Cp}\frac{dp}{dt_{chemrxn}}F_\phi(\psi,t)\right)-\frac{\partial}{\partial\psi_{S+1}}\left(\frac{h_gA}{Cp}(\psi_{S+1}-T_w)F_\phi(\psi,t)\right)+\frac{\partial}{\partial\psi_{S+1}}\left(V\frac{1}{Cp}\frac{dp}{dt_{heattransfer}}F_\phi(\psi,t)\right)$$

3. Modeling of CI Engines

In the present work, a simple mathematical model based on first principles is developed for predicting combustion characteristics in a compression ignition (CI) engine. Existing literature cites that the rate of combustion of the fuel is predicted using Wiebe function [1]. In contrast, this work involves the use of kinetic expressions for the different species like fuel (diesel – n-heptane) and other products of combustion namely, CO, CO_2, NOx. The model derivation follows our earlier work on SI engines [3].

$$C_7H_{16}+7.5O_2\rightarrow 7CO+8H_2O \tag{1}$$
$$\mathrm{CO}+\frac{1}{2}O_2\Leftrightarrow CO_2$$

A two step global kinetic expression is used assuming n-heptane (C_7H_{16}) as the species that represents diesel fuel [4], as shown in Equation (1). The combustion kinetics is coupled with the extended Zeldovich mechanism [1] to provide kinetics for NOx formation.

The summary of model equations that represent the engine model is presented here:

$$\frac{dV}{d\theta} = \frac{V_d}{2}\sin\theta\left[1 + \frac{\cos\theta}{\sqrt{R^2 - \sin^2\theta}}\right] \tag{2}$$

$$\frac{dT}{d\theta} = \frac{1}{3nC_p}\left(\sum_{j=1}^{3} v_{ij} r_j\right)\frac{V}{\omega} - \frac{P}{nC_V}\frac{dV}{d\theta} - \frac{B\omega}{nC_V} \tag{3}$$

$$\frac{d\omega}{d\theta} = \frac{\tau_{\text{Comb}}}{\text{J}\omega} - \frac{B}{J} \tag{4}$$

$$\frac{dn_i}{d\theta} = \left(\sum_{j=1}^{nrns} v_{ij} r_j\right)\frac{V}{\omega}$$

where

$$v_{ij} = \begin{bmatrix} -1 & -7.5 & 7 & 0 & 8 \\ 0 & -0.5 & -1 & 1 & 0 \\ 0 & 0.5 & 1 & -1 & 0 \end{bmatrix} \tag{5}$$

$$r_j = \begin{bmatrix} \mathrm{r}_{\text{heptane}} = 5.11\times10^{11}\mathrm{e}^{\left(\frac{-30000}{\mathrm{RT}}\right)}[\mathrm{C}_7H_{16}]^{0.25}\ [\mathrm{O}_2]^{1.5} \\ \mathrm{r}_{\text{CO-forward}} = 1\times10^{14.6}\mathrm{e}^{\left(\frac{-40000}{\mathrm{RT}}\right)}[CO]^1\ [\mathrm{H}_2O]^{0.5}[\mathrm{O}_2]^{0.25} \\ \mathrm{r}_{\text{CO-reverse}} = 5\times10^{8}\mathrm{e}^{\left(\frac{-30000}{\mathrm{RT}}\right)}\ [\mathrm{CO}_2]^{1.0} \end{bmatrix}$$

$$\frac{dn_{NO}}{d\theta} = 7.6\times10^{10}\exp\left(-\frac{30000}{T}\right)[O][N_2]\frac{V}{\omega} - 1.6\times10^{10}[NO][N]\frac{V}{\omega}$$
$$+6.4\times10^{6}T\exp\left(-\frac{3150}{T}\right)[N][O_2]\frac{V}{\omega} - 1.5\times10^{6}T\exp\left(-\frac{19500}{T}\right)[NO][O]\frac{V}{\omega} \tag{6}$$

where

$$[N] = \frac{7.6\times10^{10}\exp\left(-\frac{38000}{T}\right)[O][N_2] + 1.5\times10^{6}T\exp\left(-\frac{19500}{T}\right)[NO][O]}{1.6\times10^{10}[NO] + 6.4\times10^{6}T\exp\left(-\frac{3150}{T}\right)[O_2]}$$

where, R is the ratio of the connecting rod length (*l*) to the length of connecting rod (*a*), V_d is the displacement volume, B and J represent Friction factor and Moment of Inertia respectively. These equations coupled with initial conditions and physical engine parameters are then solved in MATLAB using solvers for stiff ordinary differential equations. EGR is defined as the fraction of exhaust that is recycled back to the inlet [5]. In the current study, cold synthetic EGR is used to study its effect on NO_X control. In other words, the feed entering the engine is modified - a fraction of fresh air is substituted with CO_2 from the exhaust in order to represent EGR. Although the actual exhaust composition is available in our simulations, and could have been used to update the inlet feed, we have chosen this simplified version of EGR for now, in order to gain insight. The results are presented in the following section.

4. Results and Discussion

The simulations are run for the engine specifications shown in literature [6]. The start of the compression stroke marks the commencement of the simulation. The results are first validated by comparing simulated pressure profiles with an experimental one from literature [6], with no EGR. The peak pressure occurs at CAD 9.52° After Top Dead Center (ATDC) and is nearly 6800 kPa. The results match agreeably with experimental data.

Figure 2 shows variation of exit NOx concentration with percent EGR. Increasing the EGR fraction lowers the peak NOx.. This is attributed to the change in composition brought in by the addition of CO_2 as synthetic EGR, replacing fresh feed. The presence of additional CO_2 changes the rate of NO formation in the engine, and we obtain lower NOx. The effect of reduction of NOx seen here is a pure inlet compositional effect, as the peak temperature is unchanged in these simulations. Furthermore, the NOx emission ppm is seen to be fairly high even with EGR, indicating that aftertreatment devices will have an important role to play at these conditions.

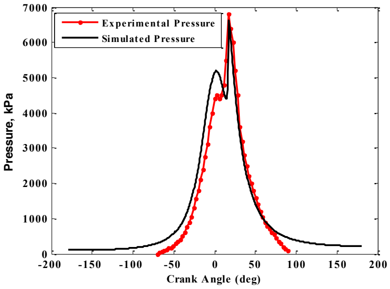

Fig. 1. The in-cylinder pressure measured in literature experiments [6] at various CAD is compared with that predicted by simulations (this work). A good match between the two serves as a validation of the proposed model .

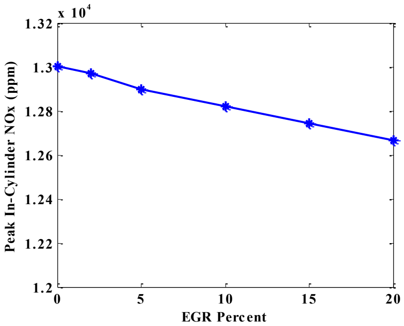

Fig. 2. The peak in-cylinder NOx (in ppm) is plotted against the %EGR, as predicted by the simulations

HCCI simulations were also carried out at various EGR percentages and equivalence ratios [7]. Similar trend of reduction in NOx with increase in %EGR was seen in these simulations.

5. Conclusions and Future Scope

A simplified model was developed based on first principles for fuel combustion in diesel engines. The model was validated against literature experimental data and good agreement observed. EGR shows synergistic effect on NOx control although currently the temperature is insensitive to EGR in the model as this point, and this feature needs to be revisited. The effect of EGR could be understood as reducing the load on the aftertreatment device, at the conditions examined here.

References

[1] Heywood, J. B., Internal Combustion Engine Fundamentals, McGraw Hill Inc., New York, 1988.

[2] DARS Manual Book 3 Engine In-cylinder Models. 2012

[3] Pratheeba, C. N., Preeti Aghalayam, Kannan Moudgalya, Sudheer Kumar Boppana, “Low dimensional modeling of combustion in SI Engines”, ***SAE*** 2013 - 23 – 0045, 2013.

[4] Westbrook, C. K., and Dryer, F. L., “Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames”, Combustion Science and Technology, Vol. 27, pp 31 - 43, 1981.

[5] Zheng, M., Reader, G. T., and Hawley, G., “Diesel engine exhaust gas recirculation – a review on advanced on novel concepts”, Energy Conversion and Management, Vol. 45, pp883-900, 2004.

[6] Sadanand Bhosle, “Dynamic Modeling and Control of Diesel Engines”, M.Tech Dissertation, IIT Bombay, 2007.

[7] C N Pratheeba and Preeti Aghalayam, “System Wide Modeling of HCCI Engine with After treatment”, 2013 AIChE Annual Meeting, San Francisco, USA, 2013.