

Numerical Investigation of a Gasoline-Like Fuel in a Heavy-Duty Compression Ignition Engine Using Global Sensitivity Analysis

Pinaki Pal

Argonne National Laboratory

Daniel Probst

Convergent Science Inc.

Yuanjiang Pei

Aramco Research Center

Yu Zhang

Aramco Services Co.

Michael Traver

Aramco Research Center

David Cleary

Aramco Services Co.

Sibendu Som

Argonne National Laboratory

ABSTRACT

Fuels in the gasoline auto-ignition range (Research Octane Number (RON) > 60) have been demonstrated to be effective alternatives to diesel fuel in compression ignition engines. Such fuels allow more time for mixing with oxygen before combustion starts, owing to longer ignition delay. Moreover, by controlling fuel injection timing, it can be ensured that the in-cylinder mixture is “premixed enough” before combustion occurs to prevent soot formation while remaining “sufficiently inhomogeneous” in order to avoid excessive heat release rates. Gasoline compression ignition (GCI) has the potential to offer diesel-like efficiency at a lower cost and can be achieved with fuels such as low-octane straight run gasoline which require significantly less processing in the refinery compared to today’s fuels.

To aid the design and optimization of a compression ignition (CI) combustion system using such fuels, a global sensitivity analysis (GSA) was conducted to understand the relative influence of various design parameters on efficiency, emissions and heat release rate. The design parameters included injection strategies, exhaust gas recirculation (EGR) fraction, temperature and pressure at intake valve closure and injector configuration. These were varied simultaneously to achieve various targets of ignition timing, combustion phasing, overall burn duration, emissions, fuel consumption, peak cylinder pressure and maximum pressure rise rate. The baseline case was a three-dimensional closed-cycle computational fluid dynamics (CFD) simulation with a sector mesh at medium load conditions. Eleven design parameters were considered and ranges of variation were prescribed to each of these. These input variables were perturbed in their respective ranges using the Monte Carlo (MC) method to generate a set of 256 CFD simulations and the targets were calculated from the simulation results. GSA was then applied as a screening tool to identify the input parameters having the most significant impact on each target. The results were further assessed by investigating the impact of individual parameter variations on the targets. Overall, it was demonstrated that GSA can be an effective tool in understanding parameters sensitive to a low temperature combustion concept with novel fuels.

CITATION: Pal, P., Probst, D., Pei, Y., Zhang, Y. et al., "Numerical Investigation of a Gasoline-Like Fuel in a Heavy-Duty Compression Ignition Engine Using Global Sensitivity Analysis," *SAE Int. J. Fuels Lubr.* 10(1):2017, doi:10.4271/2017-01-0578.

INTRODUCTION

The transportation industry accounts for around 20% of the total energy consumed globally [1]. It is expected that the global demand for transport energy will rise by ~40% by 2040. Moreover, in the foreseeable future, internal combustion (IC) engines using liquid fuels made from petroleum are expected to dominate the transport sector [2, 3, 4, 5, 6]. Given the focus on reducing greenhouse gas (GHG) emissions in the transportation industry, there is a need for more efficient IC engines for both passenger and commercial applications. This pursuit of higher efficiency has led to a stronger interest in advanced compression-ignition (CI) engines. CI engines are more fuel-efficient than the spark-ignited (SI) engines due to their relatively high compression ratios and lack of throttling losses. However, conventional CI engines suffer from higher emissions of nitrogen oxides (NO_x) and particulate matter (PM) due to local fuel-rich combustion and higher in-cylinder temperatures. Modern diesel engines use exhaust gas recirculation (EGR) to lower the in-cylinder temperature and oxygen content so that NO_x is reduced. However, this adversely affects the oxidation of any soot that is formed in the cylinder.

To address the combined needs of further emissions reduction, improved efficiency and cost, alternative forms of CI combustion are being explored [7, 8]. Gasoline compression ignition (GCI) [9] is one of the most attractive alternative combustion strategies, and can use fuels in the gasoline auto-ignition range ($\text{RON} > 60$) instead of a diesel fuel in a CI engine. The longer ignition delay of such fuels allows more time for mixing before combustion starts [10, 11, 12]. In addition, sufficient inhomogeneity in the fuel-air mixture can be ensured by late fuel injection so that combustion will occur somewhere in the cylinder and will promote combustion of the rest of the charge. At the same time, the in-cylinder mixture is “homogeneous enough” everywhere in the cylinder before combustion starts so that soot formation is circumvented [8]. Therefore, GCI has the potential to offer diesel-like efficiency at lower cost by using low-octane, low-cetane, gasoline-like fuels that may require less processing in the refinery compared to today’s fuels. Utilization of such fuels could lead to significant energy savings in fuel manufacturing. In addition, the fuel injection pressures need not be as high as with diesel fuel [13, 14, 15] as longer fuel ignition delay already facilitates better mixing. This can reduce the cost of the fuel injection system for GCI.

However, GCI combustion is dependent on a number of engine design parameters such as fuel injection strategies, EGR levels, intake temperature and pressure, and injector configuration. Different combinations of these parameters can lead to a variety of combustion characteristics, emissions and pressure rise rates. Engine simulation is a valuable tool that can aid the development of advanced combustion strategies such as GCI. Computational fluid dynamics (CFD) is being commonly used in the industry, thereby serving to shorten product development cycle and delivering significant cost savings as compared to experimental prototyping.

The influence of a large number of input parameters on specific targets of interest can be assessed using sensitivity analysis. Sensitivity analysis has been used in the chemical kinetics community as a technique for uncertainty quantification [16, 17, 18]. The goal in these studies was to identify reactions in large chemical kinetic mechanisms which influenced the ignition delay timing the most, so that the rate constants for those reactions could be computed with greater fidelity. This, in turn, led to the development of improved and more predictive chemical kinetic mechanisms.

In the past, diesel engine simulations have employed the local sensitivity analysis method to study the effect of a few parameters sequentially such as spray breakup and combustion model constants [19] to provide a guideline on how to calibrate the models under these conditions. However, this approach inherently cannot incorporate any non-linear effects. In this regard, global sensitivity analysis (GSA) has significant advantages over the traditional local sensitivity analysis approaches such as brute force methods [20]. It provides a more realistic picture by accounting for the uncertainties in all the relevant parameters considered simultaneously. Moreover, it captures the non-linear response of targets to the input parameters. Pei et al. [21] applied global sensitivity analysis to an engine simulation for the first time to quantify the sensitivities of various target functions such as ignition delay, combustion phasing and emissions to various inputs such as experimental boundary conditions, fuel properties and CFD model constants. Later, Pei et al. [22] carried out a similar study using GSA to quantify the uncertainties for the Engine Combustion Network (ECN) Spray A [23]. More recently, Kodavasal et al. [24, 25] explored the effect of uncertainties in experimental boundary conditions and fuel properties on GCI operation with conventional gasoline fuel using a similar approach for a light-duty engine. These studies demonstrated that GSA could be employed as a valuable tool to readily identify important parameters which have the greatest influence on engine combustion behavior. However, the engine combustion sensitivity to various design parameters when utilizing a low-octane gasoline-like fuel is expected to be different and hasn’t been explored previously.

Therefore, in the present work, GSA was applied to CFD simulation of a heavy-duty CI engine at medium load conditions operating with a low-octane gasoline-like fuel. A number of key design parameters are considered and their relative influences on specific targets of efficiency, emissions and heat release rate are quantified. The main objective is to provide direction on which control variables have the highest impact on the combustion characteristics, thereby requiring the highest attention during engine design and optimization phase. The paper is arranged as follows. Firstly, the engine setup is briefly discussed and details of the numerical model are provided. This is followed by a brief overview of the GSA methodology employed in this work. Next, the input parameters and their respective ranges of variation are prescribed. Then, the CFD model setup is validated against experimental data. Subsequently, the results of the GSA are discussed in terms of the sensitivity of target variables to the input parameters. Brute force sensitivity analysis is also performed on some important variables to gain additional insights. The paper concludes with a summary of the main findings.

METHODOLOGY

Engine Setup

The experimental data were generated using a four-stroke, six-cylinder, heavy-duty Cummins test engine with a variable-geometry turbocharger, high-pressure cooled EGR loop and charge air cooler. A nine-hole mini-sac injector nozzle was used. The details of the engine geometry and operating conditions for the baseline case on which the GSA was performed are listed in Table 1. The in-cylinder pressure and emissions data were used to validate the CFD model described in the next section.

Table 1. Engine specifications and operating conditions.

Engine model	Cummins ISX15
Cylinders	6
Displacement	14.9 l
Bore	137 mm
Stroke	169 mm
Connecting Rod	262 mm
Compression ratio	17.3:1
Engine speed	1375 rpm
Intake valve closing	-137 °CA aTDC
Exhaust valve opening	148 °CA aTDC
Start of injection timing	-9 °CA aTDC
Injection duration	15.58 °CA
Mass of fuel injected	0.1245 g/cycle/cylinder
Fuel injection temperature	360 K
Injection pressure	1600 bar
Nozzle inclusion angle	152°
IVC pressure	323 K
IVC temperature	2.15 bar
EGR	41%
Global equivalence ratio	0.57

Numerical Model Setup

A commercial 3-D CFD code, CONVERGE (version 2.3.8) [26], is used to perform numerical simulations for the closed part of the cycle, from intake valve closing (IVC) to exhaust valve opening (EVO). Assuming axisymmetry, the simulation domain is considered to be a sector mesh representing a single cylinder and accounting for only one spray plume in order to reduce the computational expense. Periodic boundary conditions are imposed in the azimuthal direction. A uniform mixture and temperature distribution is specified at IVC.

CONVERGE uses a modified, cut-cell Cartesian method for grid generation directly during runtime. In addition, it has the capability to include fixed embedding of cells, i.e., increasing the grid resolution with respect to base grid size *a priori* along the cylinder walls and near the nozzle, and adaptive mesh refinement (AMR) to refine areas where the sub-grid field is largest [26]. In the present work, a base mesh size of 1.4 mm is used. One level of fixed embedding is prescribed near the cylinder head and piston, while two levels of fixed embedding are employed to resolve the flow near the fuel injector. In addition, two

levels of AMR are employed based on the velocity and temperature sub-grid scales of 1 m/s and 2.5 K, respectively. This results in the minimum grid size of 0.35 mm. The computational mesh for the baseline case at top-dead-center (TDC) is shown in Figure 1. The simulation time step is automatically adjusted in the simulations based on the maximum convective, diffusive and mach Courant-Friedrichs-Lewy (CFL) numbers of 1, 2 and 50, respectively.

In-cylinder turbulence is modeled using the Reynolds-Averaged Navier Stokes (RANS) based re-normalized group (RNG) k - ϵ model [27] with wall functions. The liquid spray is treated in a Lagrangian fashion and the “blob” injection model by Reitz and Diwakar [28] is used, which initializes the diameter of a liquid droplet to the effective nozzle diameter. The Kelvin Helmholtz (KH) – Rayleigh Taylor (RT) breakup model [29, 30] and “no-time counter” collision model of Schmidt and Rutland [31] are employed to describe the subsequent spray atomization and collision processes, respectively. Droplet evaporation is modeled using Frossling correlation [32] and models are also included for dynamic drop drag [33] and droplet turbulent dispersion [34]. A reduced chemical kinetic mechanism for primary reference fuel (PRF) consisting of 48 species and 152 reactions based on Liu et al. [35] is used in this work. A RON70 two-component surrogate comprising of 70% iso-octane by mass and 30% n-heptane by mass is employed [36]. In addition, the NO_x formation is modeled by the extended Zel’dovich mechanism [37]. The empirical Hiroyasu soot model [38] coupled with the Nagle and Strickland-constable model [39] are used to determine the soot formation and oxidation rates and acetylene (C_2H_2) is considered as the precursor for soot formation. For combustion modeling, the SAGE detailed chemistry solver [40] is employed along with a multi-zone (MZ) approach, with bins of 5 K in temperature and 0.05 in equivalence ratio [26, 41]. Although it doesn’t utilize an explicit turbulent combustion closure [42, 43, 44], the SAGE-MZ model has been demonstrated to perform well to simulate spray combustion in the context of RANS in some previous studies [45].

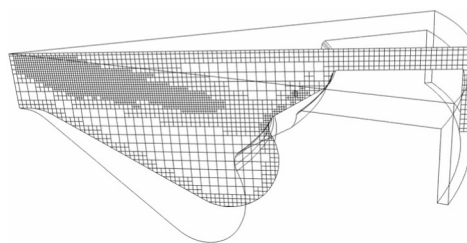


Figure 1. Computational mesh for the baseline case at TDC.

GSA Methodology

GSA is used as a tool to explore the relations between the input parameters and the outputs/targets of a model. This approach is more insightful than the local sensitivity analysis methods [46], where only a single input parameter is varied, as it captures the relative sensitivity of different variables on the targets of interest over the whole input parameter space. In doing so, it also accounts for the non-linear response of targets to the input variables. The details of the GSA methodology can be found in Ref. [16]. However, a brief discussion is provided as follows.

Assume that there are ‘ n ’ input parameters and each one of them is equally likely to lie anywhere within a prescribed range of variation:

$$v_i \in [v_i^L, v_i^H], i = 1, 2, \dots, n, \quad (1)$$

where v_i is the i th variable, v_i^L and v_i^H are the lower and higher limits of its range of variation, respectively. It is assumed that the probability distribution of the parameters is uniform within the n -dimensional hypercube [16]:

$$\Omega \in [v_1^L, v_1^H] \otimes \dots \otimes [v_i^L, v_i^H] \otimes \dots \otimes [v_n^L, v_n^H] \quad (2)$$

The Monte Carlo method is used to generate a large number ‘ N ’ of independent random parameter sets within the above hypercube for CFD simulations. In the present study, 256 simulations are used, i.e., $N = 256$. The targets obtained from the simulations can be written as:

$$f = f(v), \quad (3)$$

where f is the vector of targets of interest and v is the vector containing one set of the sampled n input parameters. The GSA is implemented based on the analysis of variance using an ordinary least squares (OLS) method through the following expansion:

$$f(v_i) = \sum_{j=1}^n \sum_{k=0}^m a_{jk} v_i^k, \quad (4)$$

where m is the order of expansion. Here, $m = 2$. The sensitivity coefficient of each input parameter (S_i) can then be computed as the ratio of the partial variance to the total variance as shown below:

$$S_i = \sigma_i^2 / \sigma_i^2, \quad (5)$$

$$\sigma_i^2 = \langle f^2 \rangle - \langle f \rangle^2, \quad (6)$$

where the brackets “ $\langle \rangle$ ” indicate the mean value over N simulations. In Eq. (5), σ_i^2 denotes the partial variance of i th parameter based on the expansion shown in Eq. (4). The larger the sensitivity coefficient, the greater the impact an input variable has on a particular target function. It must be noted that the range of variation imposed on the inputs can influence the relative values of the sensitivity coefficients.

Control Variables and Their Ranges

The design parameters used as control variables in the present study along with their respective ranges of variation are listed in Table 2. In total, eleven input variables are chosen pertaining to fuel injector design (number of nozzle holes, total nozzle area, nozzle inclusion angle), fuel injection strategy (injection pressure, start-of-injection (SOI) timing) and initial conditions (IVC temperature and pressure, EGR fraction, initial turbulence level and swirl). Each parameter is assigned a minimum and maximum value. The ranges of variation include the baseline conditions. The total nozzle area and initial

turbulence kinetic energy (TKE, k) are normalized with respect to the respective baseline values, therefore the baseline values are 1. Figure 2 shows the distributions generated for P_{IVC} and EGR. It is evident that these variables are randomly distributed using the MC method over the sample space identified by their ranges of variation. The other input parameters also have similar random distributions.

Table 2. Control variables and respective ranges of variation along with the baseline setup.

Variable	Description	Baseline	Min.	Max.
N_{holes}	Number of nozzle holes	9	8	10
A_{noz}	Total nozzle area	1	1	1.3
P_{inj}	Injection pressure [bar]	1600	1400	1800
SOI	Start-of-injection timing [°CA aTDC]	-9	-13	-5
θ_{noz}	Nozzle inclusion angle [°]	152	148	156
EGR	EGR fraction	0.41	0.35	0.50
T_{IVC}	IVC temperature [K]	323	323	373
P_{IVC}	IVC pressure [bar]	2.15	2.0	2.3
TKE, k	Initial turbulent kinetic energy	1	0.7	1.3
L_{turb}	Initial turbulence length scale [mm]	4.5	1	8
SR	Swirl ratio	1	1	2.4

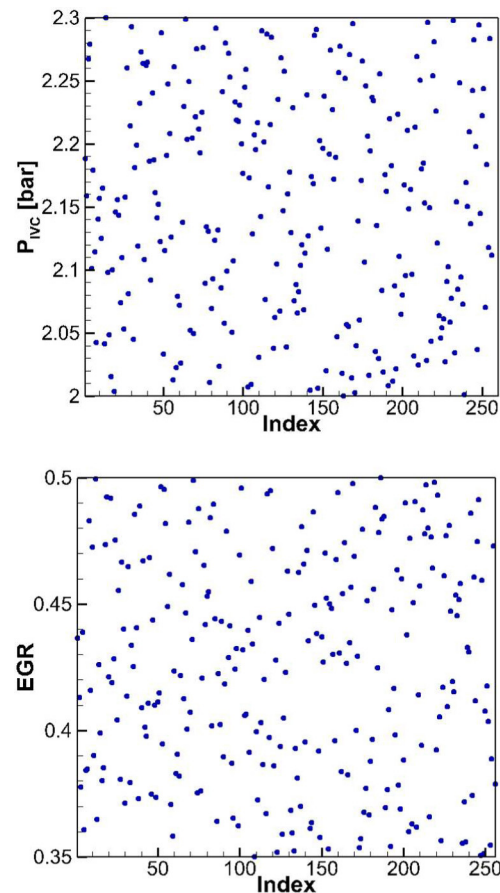


Figure 2. MC distributions of IVC pressure (top) and EGR fraction (bottom) for the 256 simulation cases.

Automated Simulation Case Setup

The initial turbulence length scale (L_{turb}) is used in the calculation of turbulent dissipation rate (ϵ in the k - ϵ turbulence model). The composition at