

# Optimization of a HSDI Diesel Engine for Passenger Cars Using a Multi-Objective Genetic Algorithm and Multi-Dimensional Modeling

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## ABSTRACT

A multi-objective genetic algorithm coupled with the KIVA3V release 2 code was used to optimize the piston bowl geometry, spray targeting, and swirl ratio levels of a high speed direct injected (HSDI) diesel engine for passenger cars. Three modes, which represent full-, mid-, and low-loads, were optimized separately. A non-dominated sorting genetic algorithm II (NSGA II) was used for the optimization. High throughput computing was conducted using the CONDOR software. An automated grid generator was used for efficient mesh generation with variable geometry parameters, including open and reentrant bowl designs. A series of new spray models featuring reduced mesh dependency were also integrated into the code. A characteristic-time combustion (CTC) model was used for the initial optimization for time savings. Model validation was performed by comparison with experiments for the baseline engine at full-, mid-, and low-load operating conditions. In addition, computations were made with a detailed chemistry combustion model to further validate the simulation results. Designs that simultaneously reduced emissions and improved fuel economy in the optimization study under different operating conditions were further analyzed. A non-parametric regression analysis tool was used to post-process the numerical results and to provide information about the effects of each design parameter on fuel economy and engine-out

emissions. The performance of these new designs was compared to the baseline engine.

## INTRODUCTION

Growing concern over environmental issues has prompted regulatory authorities to increase already stringent emission standards for the automobile industry. Meanwhile, the international crude oil price is increasing, and Green House Gases (GHG) are attracting more and more attention. Thus, fuel economy is becoming more and more important from both a customer's and a regulator's perspective. The diesel engine is an attractive option for passenger cars due to its high fuel conversion efficiency, which can be 40% more than that of modern SI engines (Cowland et al. 2004).

The current focus of engine research is on simultaneous reduction of soot and NO<sub>x</sub>, while maintaining reasonable fuel economy. Important design parameters include injection timing, injection pressure, injection rate-shape, nozzle design, swirl ratio, combustion chamber design, turbo-charging, EGR, etc. With so many engine parameters, a computational methodology for engine design is helpful to guide engine testing. A reliable and efficient CFD code for engine combustion is essential for this aim. And a fast mathematical scheme to search amongst constraint-limited objective functions for an optimum is also very important for the efficiency of the design process. Genetic algorithms have proven to be

one of the most feasible methods for engine design optimization (Shi and Reitz 2008a).

Genetic algorithm optimization is based on the idea of natural selection laws. It features a "survival of the fittest" strategy to determine the best solution to a given problem. With the genetic algorithm, each solution of the problem is viewed as an individual. The input parameters (design parameters) are the "DNA" of this individual. Part or all of the output data are used to determine the individual's chance to be selected for the next generation. Crossover and mutation operations ensure the optimality and diversity of the final Pareto front (family of optimal solutions), respectively. Genetic algorithms have been successfully used for different engine optimization tasks, when coupled with CFD models (Affes et al. 1998; Senecal and Reitz 2000; Hegarh et al. 2001; Wickman et al. 2001; Senecal et al. 2002; Shrivastava et al. 2002; De Risi et al. 2003; Subramaniam et al. 2003; Hiroyasu et al. 2004; Liu and Reitz 2005; Sun and Reitz 2006; Genzale et al. 2007; Shi and Reitz 2008a,b; Ge et al. 2009) or experiments (Thiel and Reitz 2002, Yun and Reitz 2003, 2005, Canakci and Reitz 2003, 2004). Genetic algorithm optimization was also used to calibrate the parameters in a reduced reaction mechanism (Hamosfakidis and Reitz 2003, Patel et al. 2004).

For the engine development in present work, the objectives are emissions and fuel economy. Of course, the design parameters are strongly correlated. A clear tradeoff relationship between NO<sub>x</sub> emission and fuel economy is often observed. Therefore, the use of a multi-objective genetic algorithm (MOGA) is a more feasible and efficient way for engine optimization than a single-objective genetic algorithm (SOGA).

In the present work, a diesel engine sized for passenger vehicles was optimized using MOGA and the KIVA code. Spray targeting, swirl, and 11 parameters describing the piston bowl geometry were optimized. Three different modes, which represent low-, mid-, and full-load conditions, were considered. The results were analyzed using a non-parametric regression analysis method. Sensitivities of the design parameters on the fuel economy and pollutant emissions were illustrated in response surfaces. Some of the optimum designs were further analyzed for more insights.

## OPTIMIZATION METHODOLOGIES

In terms of the number of optimization objectives, GA can be categorized as a single-objective genetic algorithm (SOGA) and multi-objective genetic algorithm (MOGA). For diesel engine combustion system development, some of the most important objectives are emissions and fuel economy. Therefore, engine optimization is naturally a multi-objective problem. Nevertheless, SOGA can still be employed for engine optimization by introducing a single merit function that combines all the objectives (Senecal and Reitz 2000;

Wickman et al. 2001; Senecal et al. 2002, Shrivastava et al. 2002; Subramaniam et al. 2003; Liu and Reitz 2005; Sun and Reitz 2006). However, these previous studies also showed that the results of SOGA depend on the definition of merit function, which is often unclear prior to the optimization process. Therefore, MOGA is getting more popular in engine optimization studies (De Risi et al. 2003, Genzale et al. 2007; Shi and Reitz 2008a,b; Ge et al. 2009).

Instead of minimizing the merit function in SOGA, MOGA searches for a so-called Pareto front, which consists of Pareto optimal designs. A Pareto design is one that no other design has better objectives. For all designs  $\vec{x}$  and the corresponding  $N$  objectives  $f_k(\vec{x})$ ,  $k = 1, 2, \dots, N$ , the Pareto design  $\vec{x}^*$  is defined as the following: for an arbitrary design  $j$ , there exists at least one objective,  $k$ , that  $f_k(\vec{x}_j) \geq f_k(\vec{x}^*)$ . The goal for the MOGA is to find the Pareto front while keeping diversity in the results.

Shi and Reitz (2008) assessed the performance of different schemes for MOGA. They concluded that a non-dominated sorting genetic algorithm II (NSGA-II, Deb et al. 2002) was the best method. Thus, we employed NSGA-II in the present work. NSGA-II employs an elite-preserving strategy and an explicit diversity-preserving mechanism. According to the objectives, elitism is given to the corresponding designs. Designs with higher elitism have priority to be selected. If two designs have the same elitism, the one with less crowding distance (proximity to other Pareto solutions) is assigned with higher priority.

Convergence of the optimization was evaluated using a simple metric (Shi and Reitz 2009), which was calculated using a method adopted from Deb and Jain (2002):

1. identify the Pareto (non-dominated) solutions of each generation that has been done. All of those Pareto solutions are combined into a pool,  $P^n$  ( $n$  is the generation number);
2. from the second generation, the Pareto solutions of the current generation can be compared with solutions in the pool that is formed by the previous generation(s) in Step 1. For each Pareto solution of the current generation, calculate the smallest normalized Euclidean distance to the solutions in the pool  $P^{n-1}$ :

$$d_i = \min_{j=1}^{N_P^{n-1}} \sqrt{\sum_{k=1}^M \left( \frac{f_{k,i} - f_{k,j}}{f_k^{\max} - f_k^{\min}} \right)^2} \quad (1)$$

$N_p^{n-1}$  is the total number of Pareto citizens of the previous generation.  $M$  is the total number of objectives.  $f_k^{\max}$  and  $f_k^{\min}$  are the maximum and minimum values of  $k$ -th objective from all  $N_p^{n-1}$  solutions in the pool  $P^{n-1}$ , respectively.

- the convergence measure is determined by averaging the normalized distance for all the Pareto citizens of the current generation:

$$C^n = \frac{1}{nn} \sum_{i=1}^{nn} d_i. \quad (2)$$

$nn$  is the total number of Pareto citizens of the current generation.

- In order to keep the convergence metric within  $[0,1]$ ,  $C^n$  is normalized by its maximum value after all generations being assigned a convergent value from Step 3::

$$\bar{C}^j = C^j / \max(C^i, i=1, \dots, n), \quad j=1, \dots, n. \quad (3)$$

Usually, the maximum value is from the beginning generations.

A non-parametric regression analysis method, Component Selection and Smoothing Operator (COSSO, Lin and Zhang 2003, Liu et al. 2006), was used to post-process all of the results including non-optimal solutions) and generate the response surfaces. COSSO is a smoothing spline analysis of variance model. The response function can be expressed as:

$$f(x) = b + \sum_{j=1}^d f_j(x^{(j)}) + \sum_{j < k} f_{jk}(x^{(j)}, x^{(k)}) + \dots \quad (4)$$

where  $b$  is constant for fitting,  $f_j$  are the main effects of each inputs,  $f_{jk}$  are the two-way interactions for each pair of input parameters, and the sequence can continue for higher order interactions. In this work, only two-way interaction was considered. The response function  $f$  is determined by minimizing:

$$\frac{1}{n} \sum_{i=1}^n [y_i - f(x_i)]^2 + \lambda J(f) \quad (5)$$

where  $y_i$  is the  $i$ -th computed data point and  $f(x_i)$  is the corresponding predicted value using Eq. (4). The role of the second term is to penalize the roughness of the response functions to avoid an excessively noisy fit, and  $J(f)$  quantifies the roughness of the response

function  $f$ . The smoothness parameter  $\lambda$  works as a weight to control the trade-off between fitting data and removing noise. The COSSO determines the penalty function from the sum of component norms and the smoothness parameter  $\lambda$ , from a cross validation technique. An iterative technique is employed to optimize the number of components to be included in Eq. (4). A design needs to be selected as the reference point of the non-parametric study. In this sense, the study can be regarded as sensitivity analysis of all parameters on the reference design of interest. After the response function has been determined, the magnitude and response shape that each design parameter will produce on the objective-space is quantified. The final response functions and response surfaces were visualized using Matlab.

## COMPUTATIONAL MODELS

An improved version of the KIVA-3V code was used for multi-dimensional modeling of engine combustion processes. It simulates the closed-valve period of the engine cycle. The turbulent flow was modeled by a modified RNG  $k-\varepsilon$  model (Han and Reitz 1995), which accounts for the effects of variable gas density in engine simulations. An improved temperature wall function model (Han and Reitz 1997) is used to predict the convective heat transfer on the solid wall. The spray breakup was modeled using the Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) model (Reitz 1987, Beale and Reitz 1999). Drop collision and coalescence were also accounted for. Spray-wall impingement was accounted for using a drop bounce-or slide model (Ricart et al. 2000). Two combustion models were used: the simplified characteristic time combustion (CTC) model and the more detailed chemistry combustion model where the CHEMKIN code is coupled with KIVA (Kong and Reitz 1993). In the CTC model, the ignition process was modeled using the Shell model (Halstead et al. 1977, Kong et al. 1995). The Shell model is able to predict the cool flame and two-stage ignition phenomena that are observed during the auto-ignition of hydrocarbon fuels through the use of a multi-step kinetics model composed of generic reactions and species. Once the defined combustion criterion temperature is reached, ignition model is switched to combustion model. The criterion temperature is set to 1000K. The CTC model, which is based on the laminar and turbulent characteristic time scales (Abraham et al. 1985, Kong et al. 1995). A two-step soot model (Hiroyasu and Kodota 1976) was used for soot prediction. The rate of soot oxidation is determined using the Nagle and Strickland-Constable model (Nagle and Strickland-Constable 1962). NO formation was calculated by the extended Zel'dovich mechanism (Bowman 1975). Recently developed gas jet model (Abani and Reitz 2007) and radius-of-influence collision model (Munnannur and Reitz 2007) were employed to reduce mesh dependency.

Previous studies (Liu and Reitz 2005, Shi and Reitz 2008) have showed that the abovementioned models are capable of capturing both combustion characteristics and emissions trends accurately, especially for traditional diesel combustion investigated in this study. Because of its relatively cheap computational cost compared to the detailed kinetic modeling, the CTC model has been extensively used in engine optimizations. However, recently Kokjohn and Reitz (2008) performed computational optimization of engine designs using detailed chemistry.

When the piston bowl geometry is optimized, the computational mesh should be generated automatically for efficiency. In the present work, the KWICK software (Wickman 2003) was used as the automated computational grid generator. KWICK adopts an iterative methodology to generate a mesh with a defined geometry and maintains the specified compression ratio. In the current study, the bowl shape is characterized using eleven parameters, including five outline parameters (the height of the central pedestal of the piston,  $A_z$ ; position of the bowl bottom,  $B_x$ ; radius of bowl,  $C_x$  and  $D_x$ ; height of point C,  $C_z$ ), and 6 other parameters for Bezier curves that connect the control points ( $X_{ab}$ ,  $X_{ba}$ ,  $X_{bc}$ ,  $X_{cb}$ ,  $Y_{cb}$ ,  $Y_{cd}$ ). The other features of the piston geometry were kept as the same as a baseline engine design. Figure 1 gives an example of grids generated by KWICK. The numbers 1–6 indicate the Bezier curve control points, which correspond to the parameters  $X_{ab}$ ,  $X_{ba}$ ,  $X_{bc}$ ,  $X_{cb}$ ,  $Y_{cb}$ , and  $Y_{cd}$ , respectively. As a compromise between computation efficiency and the model accuracy, the cell size was specified as 1 mm in this work. This resolution has been shown to give adequately mesh independent results by Abani et al. (2008).

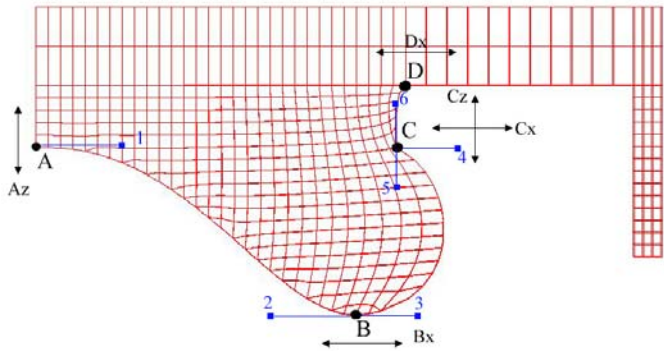


**Figure 1:** Example of grids generated by KWICK.

The KIVA-3V code and KWICK were integrated with the NSGA-II code. The optimization jobs were conducted using a high throughput computing software—Condor (Condor). Condor was designed to fully utilize distributively owned heterogeneous computing resources, which are available in the university campus<sup>①</sup>

<sup>①</sup> At the University of Wisconsin-Madison, the condor pool consists of more than 4,000 computers.

or other research communities. Like other full-featured batch systems, Condor provides a job queuing mechanism, scheduling policy, priority scheme, resource monitoring, and resource management. Condor is configured to only use idle desktop machines. When the machine is no longer available, Condor transparently produces a checkpoint and migrates the job to another idle machine. A shared file system is not necessary for Condor. Based on these features, Condor is ideal for massive computer optimization.

**ENGINE DESCRIPTION AND OPERATING CONDITIONS**

**Table 1:** Engine Specification

|                              |                         |
|------------------------------|-------------------------|
| Bore×Stroke [mm]             | 81.0×88.0               |
| Connection rod length [mm]   | 160.0                   |
| Effective ompression ratio   | 12.75:1                 |
| Fuel injector nozzles        | 8 holes, equally spaced |
| Spray pattern included angle | 153°                    |
| Nozzle orifice diameter [mm] | 0.121                   |
| IVC [°ATDC]                  | -129.5                  |
| EVO [°ATDC]                  | 120.0                   |
| Swirl ratio                  | 2.0                     |

**Table 2:** Operating conditions

|                    | Full-load | Mid-load | Low-load |
|--------------------|-----------|----------|----------|
| IMEP [bar]         | 18.0      | 15.0     | 7.0      |
| Fuel injected [mg] | 55.6      | 37.4     | 19.2     |
| RPM                | 4000      | 2400     | 1500     |
| SOI [°ATDC]        | -16       | -8       | -1       |
| DOI [°]            | 42.4      | 21.4     | 9.0      |
| EGR [%]            | 0.16      | 13.05    | 17.98    |

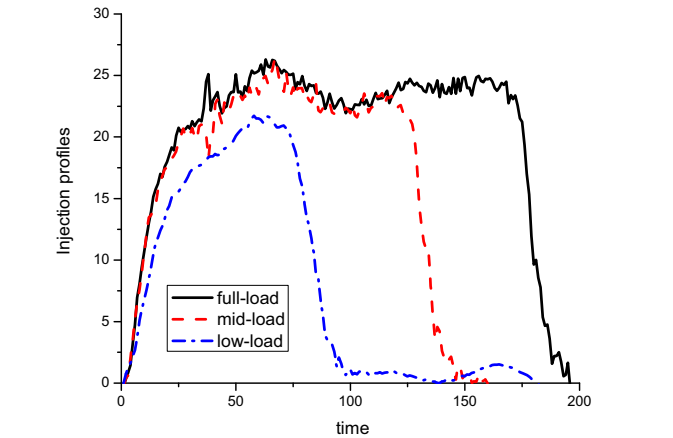


**Figure 2:** Experimental injection profiles of the full-, mid-, and low-load cases.

The engine investigated in the present work is a diesel engine for passenger vehicles. Table 1 lists the specifications of this engine. Three different operating

conditions, which represent full-load, mid-load, and low-load, respectively, were considered. The operating conditions of the three modes are detailed in Table 2. Figure 2 shows the injection profiles of the full-, mid-, and low-load cases. The injection profiles were evaluated from experimental characterization of the nozzle hardware.

## OPTIMIZATION PARAMETERS AND OBJECTIVES

Engine operation under the three modes was optimized separately. However, except for the Start-of-Injection (SOI) timing, the optimizations of the three modes had the same search space shown in Table 3. All of the parameters are set as real variables except for the number of nozzle holes, which has to be an integer. However, the integer (binary) variable is limited to a finite number of choices. In the present optimization, the total number of possibilities in nozzle hole number is 8 (5 to 12 holes). When the number of nozzle holes varies, the amount of injected fuel, injection velocity and injection duration is kept the same as the baseline engine. Thus, the total flow area of the nozzle holes is kept the same as the original value. With fewer nozzle holes, the size of nozzle hole is bigger and the initial droplet size is larger. To fully understand the influence of the design parameters, extensive search spaces were employed in the present work.

Since plenty of computer nodes are available on Condor pool, we can submit many jobs simultaneously. A large number for population size is then preferred. In the present work, the population size is set to 32, which works well and relatively big (Shi and Reitz 2008a). It usually takes about 6 to 12 hours to complete one generation.

**Table 3:** Optimization search space

|                    |           | Minimum | Maximum |
|--------------------|-----------|---------|---------|
| Spray angle [°]    |           | 140     | 160     |
| Nozzle hole number |           | 5       | 12      |
| Swirl ratio        |           | 0.5     | 2.5     |
| Az                 |           | 0.5     | 0.8     |
| Bx                 |           | 0.8     | 1.0     |
| Cx                 |           | 0.45    | 0.65    |
| Cz                 |           | 0.60    | 0.85    |
| Dx                 |           | 0.45    | 0.70    |
| Xab                |           | 0.1     | 0.7     |
| Xba                |           | 0.3     | 0.9     |
| Xbc                |           | 0.5     | 3.5     |
| Xcb                |           | 0.5     | 3.5     |
| Ycb                |           | 0.3     | 0.9     |
| Ycd                |           | 0.3     | 0.9     |
| SOI<br>[°ATDC]     | Full-load | -20     | -5      |
|                    | Mid-load  | -18     | 2       |
|                    | Low-load  | -20     | 15      |

## RESULTS AND DISCUSSIONS

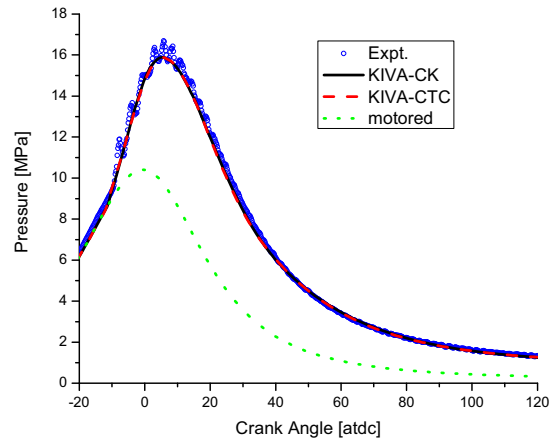


**Figure 3:** Fired and motored in-cylinder pressure of full-load baseline case.

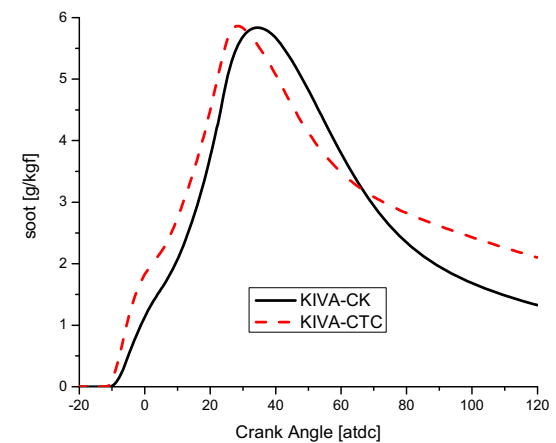
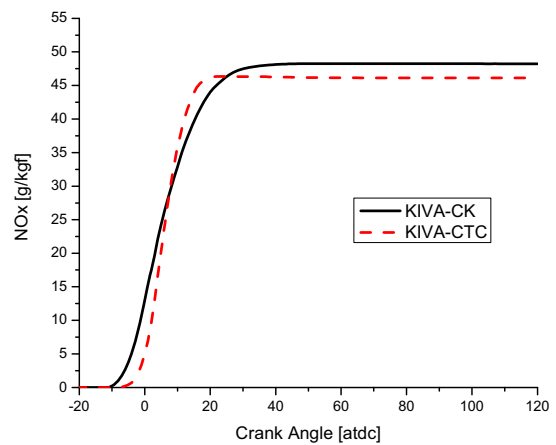


**Figure 4:** NOx (top) and soot (bottom) emissions of full-load case computed using the CTC and KIVA-CHEMKIN (CK) models.

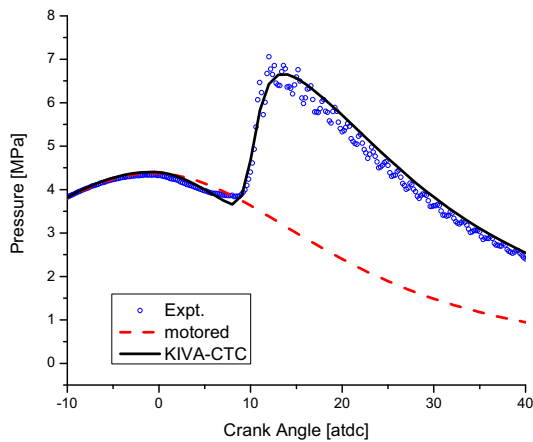
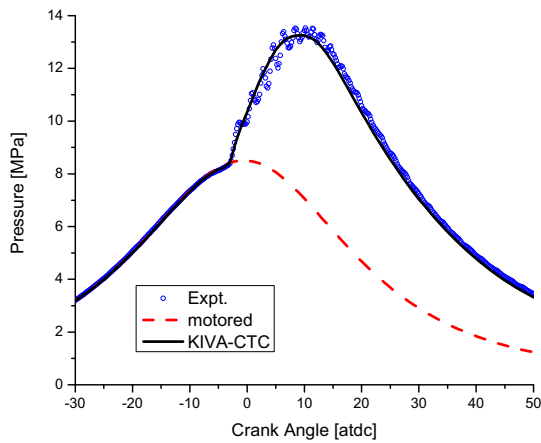


**Figure 5:** Fired and motored in-cylinder pressure of mid-load (top) and low-load (bottom) cases.

**VALIDATION OF BASELINE CASES** - The baseline full-load case was simulated using both the CTC and KIVA-CHEMKIN models. The pressure traces are plotted in Fig.3, which includes the motored case. Both the CTC and KIVA-CHEMKIN models give very good matches with the experimental data. NO<sub>x</sub> and soot emissions predicted by the CTC and KIVA-CHEMKIN models, which are shown in Fig.4, are also very close. This implies that the results of the CTC model are reliable. Since the computational cost of the CTC model is much less than the KIVA-CHEMKIN model, and many cases need to be computed to cover the design space, the CTC model was used in optimization.

The mid- and low-load cases were also validated against experimental data using the CTC model. Computed fired and motored in-cylinder pressure, as well as the measured in-cylinder pressure, is presented in Fig.5. The numerical results are in good agreement with the experimental data.

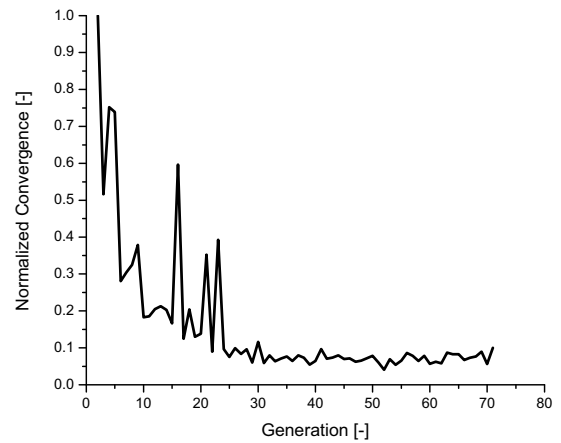


**Figure 6:** Normalized convergence history of the optimization of full-load case.

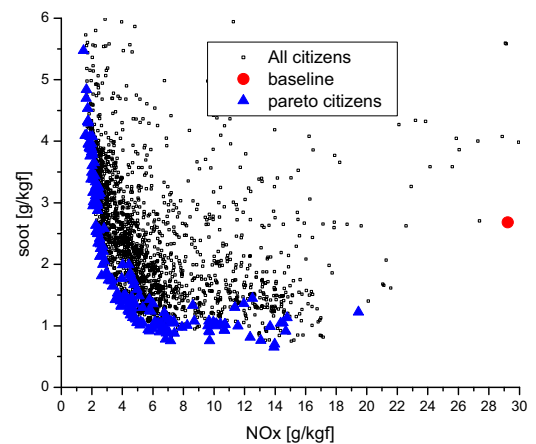
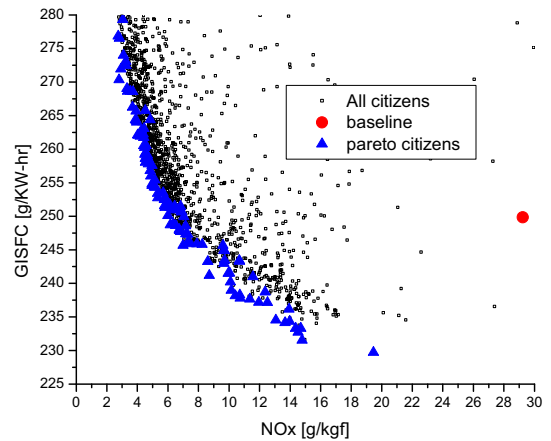


**Figure 7:** All citizens and Pareto solutions from optimization, and the baseline design for the full-load case.

OPTIMIZATION OF FULL-LOAD CASE - As proved in Shi and Reitz (2008) and Ge et al. (2009), the full-load (high-load) case is the most critical case for engine optimization. Therefore, the full-load case was optimized first. The optimization was terminated at the 72<sup>nd</sup> generation, which results in about 2300 designs. The convergence metric of this optimization was then calculated using Eqs. (1-3). Figure 6 shows the history of the normalized convergence. The convergence was reached by the 30<sup>th</sup> generation.

All the citizens, with highlighted Pareto solutions and the baseline case, are plotted in Fig. 7. Normal citizens, Pareto citizens, and baseline design are indicated by black hollow squares, blue triangles, and the red circle, respectively. The baseline engine performance is seen to be improved upon significantly in terms of all the objectives.

Figure 8 summaries the response functions of all the design parameters of the full-load case, as evaluated using the COSSO method. Their effects on the GISFC<sup>1</sup>, soot and NOx are illustrated in the left, middle, and right columns, respectively. The absolute error values of these response functions are about 10g/kW-hr, 0.7g/kgf, and 1.2g/kgf for GISFC, soot, and NOx, respectively. In general, the number of nozzle holes, which ranges from 5 to 12, has the most significant impact on the GISFC and soot emission. A nozzle with 6 to 8 holes benefits combustion efficiency and soot reduction. A nozzle with fewer holes gives lower NOx emissions. The AFR of the full-load case is about 20 (global equivalence ratio is about 0.75). Therefore, it is essential to deliver the fuel to each corner of the combustion chamber to achieve good combustion efficiency. Plus, the pressure and temperature in this case is very high, and the droplets evaporate very fast. If the initial droplet size is too small, the spray penetration will be too short for the fuel to reach the near wall squish region (which has more oxygen than the cylinder center).

A nozzle with more holes produces smaller droplets, which have shorter spray penetrations. In this case, it becomes very difficult for the fuel to mix with the oxygen near the wall and results in poor combustion efficiency.

On the other hand, if the initial droplet size is too large, it presents the risk of spray wall impingement, which will lead to poor combustion efficiency and high soot and UHC emissions. Thus, the key issue for combustion efficiency of the full-load case lies in keeping spray penetration as long as possible while avoiding spray wall

impingement. These effects of nozzle hole number (hole size) on the GISFC and pollutant emission are clearly reflected in the response functions.

SOI is the most critical parameter for NOx emissions. The NOx formation reactions are relatively slow as compared to many other elementary reactions involved in the heat release. Therefore, the total NOx emission is proportional to the total lifetime of the high temperature mixtures. Early injection usually has earlier ignition, which provides more time for NOx formation. Thus, a late injection consistently gives lower NOx emissions.

SOI also has a strong impact on the combustion efficiency. With different SOI, different percentages of fuel are injected into the bowl or squish regions. If too much fuel is injected into one region, it is very difficult to transport the abundant fuel into the other region. In this sense, the effects of SOI and spray angle on the GISFC are the same: to deliver the appropriate amount of fuel to the squish and bowl region. A SOI around -15° ATDC is seen to give the best GISFC. This implies that, with this SOI, the ratio of the fuel delivered into the squish region and the bowl region is the same as the ratio of the amount of available oxygen in these two regions.

The response functions of spray angle show that a wider spray angle simultaneously reduces fuel consumption and pollutant emissions. A wider spray delivers more fuel into the squish region where there is more oxygen. Swirl adds a tangential velocity to the flow. Therefore, it enhances the mixing in the tangential direction and this enhances the evaporation of droplets. Consequently, it further reduces the spray penetration. Thus, for the same reason as the effects of nozzle hole number, strong swirl reduces GISFC. Too weak a swirl leads to poor mixing between fuel and oxygen in the tangential direction, and eventually to poor combustion efficiency. The best fuel consumption is achieved when the swirl ratio is around 1.8. Note that strong swirl always benefits the soot reduction. However, a clear tradeoff between fuel consumption and NOx formation is observed in terms of the effects of the swirl flow.

The design parameters of the piston bowl can be separated into two categories: (1) outline parameters; and (2) Bezier curvature parameters. Among the five outline parameters (Az, Bx, Cx, Cz, and Dx), Cx is the most important one in terms of their impact on GISFC and pollutant emissions. Cx is the primary parameter defining the radius of the piston bowl. It can be seen that  $Cx \approx 0.6$  gives the best GISFC and soot emissions, while keeping NOx emissions at an acceptable level. Since the position of point C is very important at full-load, the bowl curvature about point C becomes very important as well. One of its curvature parameters, Xbc, is seen to be the most important Bezier curvature parameter for GISFC and pollutant emissions. The curvature parameters have strong effects on the flow pattern in the piston bowl, especially the tumble flows. Therefore, their impacts on soot emission are more evident than on the

<sup>1</sup> GISFC refers to the work delivered to the piston over compression and expansion strokes, i.e., from BDC to TDC to BDC. In the present work, "GISFC" is defined as the output work from IVC to EVO for convenience. Apparently, there is a difference between these two "GISFC". This difference is a constant for the same engine and same operating conditions. Therefore it will not affect the results and conclusions.