

An Investigation of the Gradient Determination Strategies for the Optimization of Diesel Engines.

Seshasai Srinivasan* and Franz X. Tanner

Institute for Computational Science and Engineering, Michigan Technological University, Houghton, MI 49931-1295

ABSTRACT

The main objective of this study is to determine an accurate and computationally efficient gradient approximation method for gradient-based algorithms used in engine optimizations. The forward difference and the central difference approximation schemes have been explored by optimizing the split injection timings for a Sulzer-S20 diesel engine. The analysis has been carried out for two different starting points, and the optimization processes suggest that both methods yield the same optimum for the respective starting points. Since the central difference scheme generally requires more function evaluations, this study proposes that the forward difference approximation is a sufficiently accurate method for estimating the gradients.

INTRODUCTION

Over the years, several engine operating parameters and design variables that influence the emissions and fuel consumption have been identified and studied. Among these, split-injection techniques (c.f. [1–5]), often in combination with exhaust gas recirculation (EGR) (e.g. [6–9]), have been investigated in several experimental and computational studies.

These studies have indicated that these and many other parameters are linked in a complex manner. Therefore, optimizing an engine with respect to emissions and low fuel consumption requires a search over a high dimensional parameter space. This search is further complicated by the notorious trade-offs between emissions, viz., soot (PM) and nitric oxide (NO_x), and the specific fuel consumption (SFC). Normally, a reduction in soot occurs at the expense of NO_x and vice versa. Also, a reduction in NO_x is generally at the expense of the SFC.

The search for optimal engine operating conditions requires minimizing an appropriate cost function on a higher dimensional parameter space. The inputs for the cost function, i.e. the emissions and SFC values, are obtained from a time intensive CFD based engine simulation. Therefore, the optimization tool must be computationally very efficient, requiring as few function evaluations as possible to reach an optimal solution.

Currently, there are two popular optimization methods used for engine optimizations: a heuristic approach based on the genetic algorithm (GA) (c.f. 10–13), and gradient-based methods (c.f [9, 14, 15]). GAs mimic the principle of natural selection, whereas gradient methods take a more

deterministic approach. This study focuses on the latter.

The gradient-based algorithms perform a systematic search in a particular direction to obtain an optimal solution to the given problem. Unlike GAs, these methods are computationally very efficient because they require fewer cost function evaluations, i.e., engine simulations, to reach an optimum. However, gradient methods are less likely to find a global optimum, since they can get stuck at a local minimum.

In gradient methods, the correct computation of the search directions is critical for their success. In previous studies by these authors (c.f [9, 14, 15]), a forward difference scheme has been used to approximate the gradient at a pivot. The purpose of the present study is to show that the forward difference scheme is sufficient. Therefore, the more accurate but computationally more expensive central difference scheme has been utilized and its results are compared with the ones obtained from the forward difference scheme.

The two gradient-determining approaches are used for the optimization of the split injection timings of a Sulzer-S20 (S20) diesel engine. The optimization parameters include the start of injection of the first pulse, the durations of the two pulses and the duration of the dwell. The engine simulations were performed with a modified version of the multi-dimensional CFD code *KIVA-3*.

OPTIMIZATION

The optimization approach taken in this study is based on the steepest descent method which utilizes an adaptive cost function in conjunction with a backtracking strategy for the line search. The backtracking algorithm makes use of quadratic and cubic polynomials to accelerate the conver-

*Corresponding author. stsriniv@mtu.edu

gence, and the initial backtracking step employs an adaptive step size mechanism which depends on the steepness of the search direction. Further, the parameter space, $\bar{X} \subset \mathbb{R}^m$, has been normalized to be the unit hypercube, where m is the number of parameters.

The Adaptive Steepest Descent Method

In each iteration step, k , the steepest descent method determines a search direction, $p_k = -\nabla f(x_k; \zeta_k)$, at the pivot, x_k , where ζ_k is the penalty parameter and the gradient, ∇ , is taken with respect to the (normalized) parameter x . The cost function f is then minimized along this search direction, using the backtracking algorithm described below. This minimization process, called line search, yields a new pivot x_{k+1} and a new penalty parameter ζ_{k+1} , which allows the determination of the new search direction p_{k+1} . This iteration process is continued until either the target is reached or a minimum is encountered. The algorithm for this adaptive steepest descent method is given in [9].

The Backtracking Method

The backtracking algorithm used in this study is a modified version of the one presented in [16]. It is equipped with an additional adaptive initial step size for the first backtracking step and minimizes either a quadratic or a cubic polynomial to find the subsequent step sizes and hence the new pivot x_{k+1} . Note that during the backtracking phase the penalty parameter ζ remains constant. The details of this algorithm are described in [9].

The Cost Function

The cost function is a measure for the quality of a particular engine operating point. The smaller the cost function, the lower the SFC and the closer the emissions are to the targets. In the present study, the cost function used is based on the penalty method, and is given by

$$f(x; \zeta) = \frac{S}{2} \left(\frac{SFC}{SFC_0} \right)^s + \frac{\zeta}{2} \left(C \left| \frac{PM - PM_0}{PM_0} \right|^c + N \left| \frac{NOx - (NOx)_0}{(NOx)_0} \right|^n \right).$$

The penalty parameter, ζ , is updated at every pivot by

$$\zeta_{k+1} = S \left(\frac{SFC(x_{k+1})}{SFC_0} \right)^s / \left(C \left| \frac{PM(x_{k+1}) - PM_0}{PM_0} \right|^c + N \left| \frac{NOx(x_{k+1}) - (NOx)_0}{(NOx)_0} \right|^n \right).$$

The positive weights C , N and S , and the positive exponents c , n , and s determine the importance of each of the three quantities to be optimized. In this study, all the weights have been set to one and the exponents have the values $c = 1$, $n = 1$ and $s = 2$.

The factors PM , NOx and SFC are the values computed during the process of optimization while the values

Table 1 Engine specifications for the Sulzer S20.

Bore [mm] × stroke [mm]	200 × 300
Engine speed [rev/min]	1000
Orifices × diameter [mm]	12 × 0.285
Start of injection [CA ATDC]	-10.5
Duration of injection [CA]	32
Fuel injected [g]	1.02
Power output [KW/cylinder]	157.6

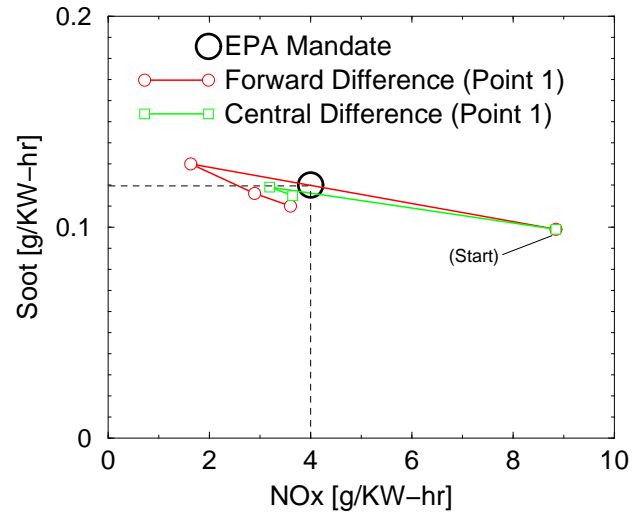


Figure 1 NOx and soot values at the pivots of the search path for the first starting point.

PM_0 , NOx_0 and SFC_0 are the target values. In this study, the target values are $PM_0 = 0.06$ g/KW-hr and $NOx_0 = 3.5$ g/KW-hr, which, for computational reasons, were chosen below the respective EPA mandates of 0.12 g/KW-hr and 4 g/KW-hr. The target value $SFC_0 = 194.13$ g/KW-hr is the one obtained from the engine tuning case (cf. [9]).

In the simulations, the SFC is computed as $SFC = \dot{m}_f / P$ where \dot{m}_f is the rate of injection of the fuel mass and the power output, P , is given as $P = \frac{RPM}{120} \int_{IVC}^{EVO} p dV - L$, where RPM is the engine speed in revolutions per minute, p is the cylinder pressure, dV is the differential volume change and L represents the power losses due to friction, scavenging and operation of peripherals like the turbocharger and the injection system. The integration is done from the closure of the inlet valves (IVC) at -144 CA after top dead center (ATDC) until the opening of the exhaust valves (EVO) at 129 CA ATDC. The difference between the experimental power output of 157.6 KW and the tuning case power output of 169.6 KW is 12 KW and is taken as the losses, L . Since the simulations are performed at full load the changes to L at different operating points are expected to be small in comparison to the power output and, therefore, this approximation will have a negligible effect on the overall optimization results.

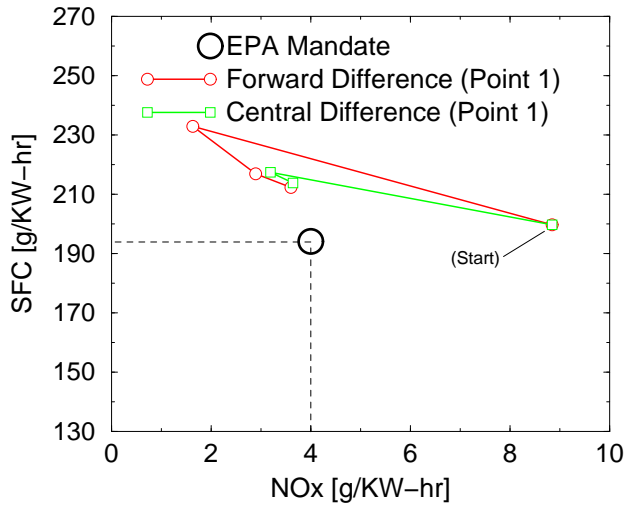


Figure 2 NO_x and SFC values at the pivots of the search path for the first starting point.

COMPUTATIONAL DETAILS

The engine computations have been done with an enhanced version of the *KIVA-3* code, which is equipped with many new or improved models whose details are given in [9].

All the computations have been done for a four-stroke Sulzer S20 DI diesel engine with a central injector equipped with 12 nozzle orifices. The main engine specifications and the tuning case operating conditions are listed in Table 1. The experimental data for the engine have been obtained from a nine-cylinder production engine and are reported in [17].

The cylinder flow is assumed to be periodic with respect to the number of nozzle orifices, and therefore, only one sector of the combustion chamber, corresponding to one nozzle orifice, was simulated. The mesh used for the simulations had $23 \times 13 \times 14$ cells in the radial, azimuthal and the vertical direction at TDC. The computations were done from the closure of the inlet valves at -144 CA ATDC to the opening of the exhaust valves at 129 CA ATDC. All simulations were performed at full load and at 1000 RPM, with 1.02 g of fuel injected using a common rail injection system.

The range of the optimization parameters are as follows. The *start of injection of the first pulse* ranges from -15 CA ATDC to 5 CA ATDC. All the other parameters lie in the range $0 - 30$ CA. Thus, in principle, one or more of the parameters could go to zero. For the computation of the gradients, the differential step size in the normalized parameter space was set to $dx_i = 2/(p_{max,i} - p_{min,i})$, $i = 1, \dots, 4$, where $p_{max,i}$ and $p_{min,i}$ are the interval endpoints of the i -th optimization parameter. Note that, in order to avoid a peak injection pressure of more than 210 MPa, the sum of the injection durations was limited to no less than 20 CA.

RESULTS AND DISCUSSION

Optimization runs have been made for the split injection at two different starting points. The influence of the central

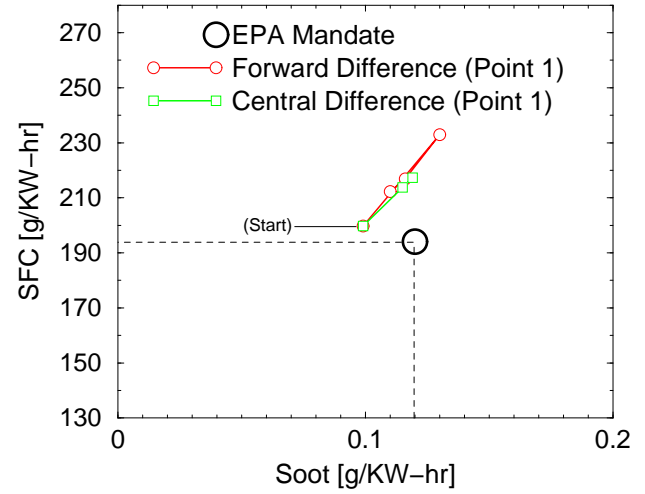


Figure 3 Soot and SFC values at the pivots of the search path for the first starting point.

difference and the forward difference approximation of the gradients on the optimal solution have been investigated for each of these points.

First Starting Point

In this case the start of injection of the first pulse was at -10.5 CA ATDC. The parameter values of the starting point and the results of the two gradient approximation schemes are summarized in Table 2. Both approaches lead to optimal points whose parameter values lie within one CA of each other. For all practical purposes, these two optimal points can be considered the same. Also, the emission and SFC values of the two optimal points are almost identical.

As is seen in Table 2, in comparison with the starting point, the optimal points have a delayed start of injection of about 1.5 CA, followed by a pilot injection of the same duration (13 CA), a dwell extended by about 2 CA and a second pulse which is longer by approximately 2.5 CA. This injection strategy results in a positive influence on the emissions. The delayed start of injection and the extended dwell move the second pulse later into the expansion stroke which decreases the peak cylinder pressures by approximately 10 bar, resulting in lower cylinder temperatures and consequently a reduced NO_x formation. The NO_x formation is further reduced by the internal EGR effect caused by the interaction of the combustion products of the first pulse with the second pulse.

The emission and SFC results of the two optimization runs are shown in Figures 1, 2 and 3. As is seen in Figure 1, both cases meet the emission mandates. This is however, at the expense of SFC which is higher than the starting point by about 7% .

As can be seen from these figures, the optimum points are very close but the paths taken by the two cases are different. This is due to the slight differences in the gradients at the starting points which may cause the line searches to lead to

Table 2 Starting and optimum data obtained from the simulations with the start of injection at -10.5 CA ATDC.

Parameters	Starting Point	Optimal Points	
		Fwd. Diff	Cen. Diff
Parameters			
SOI of first pulse [CA ATDC]	-10.5	-8.82	-9.12
Duration of 1 st pulse [CA]	13	12.54	13.6
Duration of dwell [CA]	6	8.87	7.99
Duration of 2 nd pulse [CA]	13	15.27	15.60
Engine output			
Particulates [g/KW-hr]	0.099	0.110	0.115
NOx [g/KW-hr]	8.84	3.60	3.64
SFC [g/KW-hr]	199.75	212.32	213.82
Max. cyl. pressure [MPa]	16.13	15.12	15.02
Computation			
# function evaluations		23	23

different intermediate pivots. It is interesting to note that the two gradient approaches yield different search paths but terminate at almost the same optimum.

The central difference scheme requires four more function evaluations per pivot than the forward difference scheme. However, the former case needs 3 line searches to reach the optimum whereas the latter requires only 2. The net effect is that the total number of function evaluations in both cases was 23. From this point of view it is not clear that the forward difference scheme is computationally more efficient, since a more accurate computation of the search direction with the central difference scheme results in fewer line searches. Important, however, is the fact, that the two methods yield practically the same optimum.

Second Starting Point

In the previous starting point it was observed that the two gradient strategies converged to optima that are almost identical. In order to verify that this behavior is independent of the starting point, similar optimization runs were performed for a different starting point in which the start of injection was delayed to -5.5 CA ATDC. The results of the two optimization runs for this case are summarized in Table 3. As in the previous case, both approaches lead to optimal points whose parameter values lie within one CA of each other which, for practical purposes, can be considered the same. Also, the emission and SFC values of the two optimal points are almost the same.

Once again, as seen from Table 3, at the optimum, the start of injection is slightly delayed in comparison with the starting point. This is followed by a pilot injection of about 13 CA and a dwell of about 7 CA, after which the remaining fuel is injected. Thus, the injection characteristics are very similar to the optima of the first starting point.

Both optimization runs meet the EPA emission mandates, as can be seen from Figures 4 and 6. As in the previous starting point case, the emission mandates are met at the expense

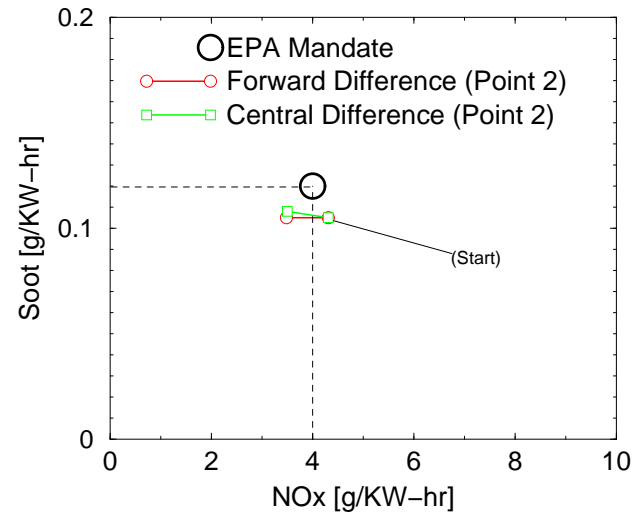


Figure 4 NOx and soot values at the pivots of the search path for the second starting point.

of SFC, which has increased by about 1.5% from the starting value of 209.94 gm/KW-hr to approximately 213 gm/KW-hr.

As before the two gradient approaches move along different search paths before they converge to nearly the same optimum. Once again, this can be attributed to a relatively flat cost function surface on which slight variations in the initial gradients can lead to different intermediate pivots. Nevertheless, the final optimal points in both optimization runs are in close agreement.

Both optimization runs required only one line search to reach the optimum. The number of function evaluations needed in the forward and central difference approaches are 8 and 12, respectively. The higher number in the latter case is solely due to the extra four computations required to determine the gradient.

Table 3 Starting and optimum data obtained from the simulations with the start of injection at -5.5 CA ATDC.

Parameters	Starting Point	Optimal Points	
		Fwd. Diff	Cen. Diff
SOI of first pulse [CA ATDC]	-5.5	-5.05	-5.26
Duration of 1 st pulse [CA]	13	13.61	13.31
Duration of dwell [CA]	6	7.12	6.48
Duration of 2 nd pulse [CA]	13	12.75	13.38
Engine output			
Particulates [g/KW-hr]	0.105	0.105	0.108
NOx [g/KW-hr]	4.30	3.48	3.56
SFC [g/KW-hr]	209.94	213.28	213.25
Max. cyl. pressure [MPa]	14.41	14.21	14.18
Computation			
# function evaluations		8	12

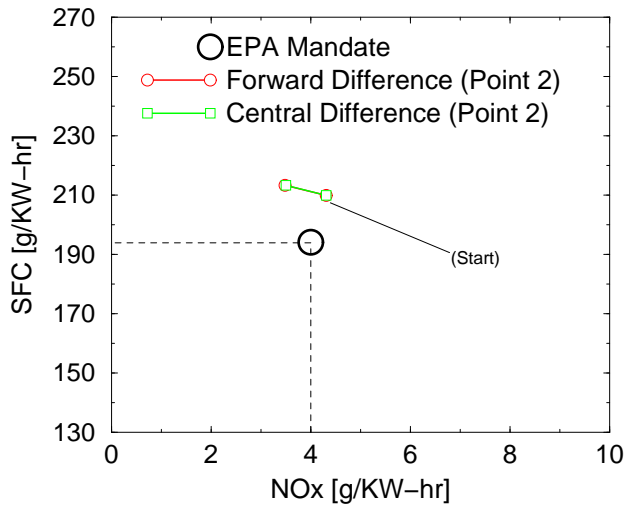


Figure 5 NOx and SFC values at the pivots of the search path for the second starting point.

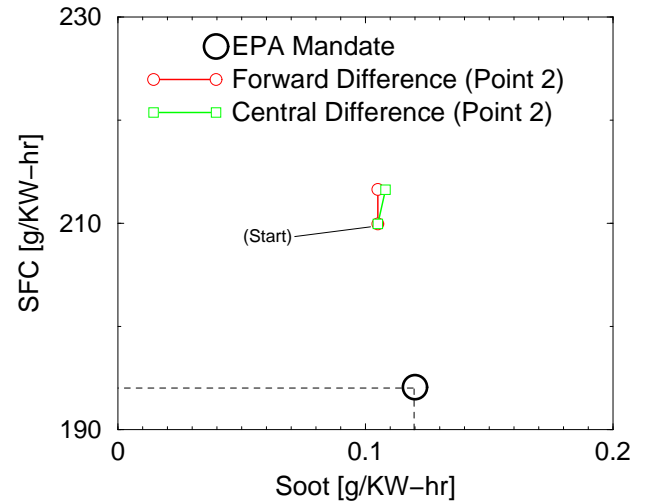


Figure 6 Soot and SFC values at the pivots of the search path for the second starting point.

Comparison Between Starting Points

On comparing the optima of the first starting point cases with the optima of the second starting point cases, we find that the start of injection in the latter cases are delayed by about 3 CA. This is compensated by a corresponding shorter injection duration of the second pulse, which is approximately 14 CA.

Also, the optimal values of emissions and SFC are almost the same in all the four optimization runs. This indicates that there is probably a flat valley in one particular direction on the surface of the cost function. This might be the reason that the two different starting points lead to different optimum parameters but with almost identical emission and SFC values. This implies that there might be many operating conditions yielding the same cost values at the bottom of this valley. In other words, the global minimum might not

be unique.

With the above studies, it is evident that both gradient determination strategies, viz., forward difference approximation and the central difference approximation, yield the same optimum value for a given starting point. However, it is expected that in general the number of function evaluations might be higher in case of the central difference approximation, since twice the number of function evaluations are required at each pivot to find the search direction. Hence, it can safely be concluded that the forward difference approximation is a reasonably accurate and a less expensive gradient determination technique.

SUMMARY AND CONCLUSIONS

Two gradient determination strategies, the forward difference approximation and the central difference approximation, have been investigated to study their influence on the optimization of a Sulzer-S20 diesel engine. The techniques were applied to two different starting points of a split injection case that varied in their start of injection time.

All the four optimization cases met the EPA emission mandates. This was however at the expense of the SFC which increased to about 213 g/KW-hr in all cases. The reduction in NO_x and the marginal increase in soot was mainly due to the split injection in which the combustion of the second fuel pulse was delayed into the expansion stroke, thus avoiding high in-cylinder temperatures. Also, the internal EGR effect, created by the combustion products of the first pulse, contributed to the NO_x reduction. On the other hand, the delay in the combustion of the second pulse resulted in a lower peak cylinder pressure and hence a reduced power output, which lead to an increase in the SFC.

For all practical purposes, the optimization runs had the same emission and SFC values. This indicates that the cost function surface is likely to have a nearly flat valley along a particular direction. Further, both gradient approaches reached an almost identical optimum point for a given starting point. However, the path taken by each approach was different, i.e, the intermediate pivots in the two cases were not the same. This can be attributed to the slight differences in the initial gradients predicted by the two methods on a relatively flat cost surface.

The two optimization runs corresponding to the first starting point required as many as 23 function evaluations. The forward difference required an extra line search over the central difference case. In the two optimization runs corresponding to the second starting point, the number of function evaluations required by the central difference were larger. In view of the fact that the predicted optima are almost identical for each of the two different starting points, the forward difference approximation is proposed as a reasonably accurate and computationally efficient method of determining the gradient.

Future studies will investigate the least squares approach of determining the gradient as is typically used in response surface methods in experimental engine optimizations.

REFERENCES

1. D. Nehmer and R. D. Reitz. Measurement of the Effect of the Injection Rate and Split Injections on Diesel Engine Soot and NO_x Emissions. SAE Paper 940668, 1994.
2. M. A. Patterson, S. C. Kong, G. J. Hampson, and R. D. Reitz. Modeling the Effects of Fuel Injection Characteristics on Diesel Engine Soot and NO_x Emissions. SAE Paper 940523, 1994.
3. T. Tow, D. Pierpont, and R. D. Reitz. Reducing Particulate and NO_x Emissions by Using Multiple Injections in a Heavy Duty D.I. Diesel Engine. SAE Paper 940897, 1994.
4. A. Uludogan, J. Xin, and R. D. Reitz. Exploring the Use of Multiple Injectors and Split Injection to Reduce D.I. Diesel Engine Emissions. SAE Paper 962058, 1996.
5. N. S. Ayoub and R. D. Reitz. Multidimensional Modeling of Fuel Effects and Split Injections on Diesel Engine Cold-Starting. *Propulsion and Power*, 13:123–103, 1997.
6. D. Pierpont, D. Montgomery, and R. D. Reitz. Reducing Particulate and NO_x Using Multiple Injections and EGR in a D.I. Diesel Engine. SAE Paper 950217, 1995.
7. D. Montgomery and R. D. Reitz. Six-Mode Cycle Evaluation of the Effect of EGR and Multiple Injections on Particulate and NO_x Emissions from a D.I. Diesel Engine. SAE Paper 960316, 1996.
8. Michael Chan, Sudhakar Das, and Rolf D. Reitz. Modeling Multiple Injection and EGR Effects on Diesel Engine Emissions. SAE Paper 972864, 1997.
9. Seshasai Srinivasan, F. X. Tanner, Jan Macek, and Polacek. Milos. Computational Optimization of Split Injections and EGR in a Diesel Engine Using an Adaptive Gradient-Based Algorithm. SAE Paper 2006-01-0059, 2006.
10. Michael J. Bergin, Randy P. Hessel, and Rolf D. Reitz. Optimization of a large diesel engine via spin spray combustion. SAE Paper 2005-01-0916, 2005.
11. Manshik Kim, Mike P. Liechty, and Rolf D. Reitz. Application of micro-genetic algorithms for the optimization of injection strategies in a heavy-duty diesel engine. SAE Paper 2005-01-0219, 2005.
12. Yi Liu and Rolf D. Reitz. Optimizing HSDI diesel combustion and emissions using multiple injection strategies. SAE Paper 2005-01-0212, 2005.
13. A. de Risi, T. Donato, and D. Laforgia. Optimization of the Combustion Chamber of Direct Injection Diesel Engines. SAE Paper 2003-01-1064, 2003.
14. F. X. Tanner and Seshasai Srinivasan. Optimization of Fuel Injection Configurations for the Reduction of Emissions and Fuel Consumption in a Diesel Engine Using a Conjugate Gradient Method. SAE Paper 2005-01-1244, 2005.
15. F. X. Tanner and Seshasai Srinivasan. Gradient-Based Optimization of a Multi-Orifice Asynchron Injection System in a Diesel Engine Using an Adaptive Cost Function. SAE Paper 2006-01-1551, 2006.
16. J. Dennis and R. B. Schnabel. *Numerical Methods for Unconstrained Optimization and Nonlinear Equation*. Prentice Hall, Englewood Cliffs, N.J., 1983.
17. H. Stebler. *Luft- und brennstoffseitige Massnahmen zur internen NO_x-Reduktion von schnelllaufenden direkteingespritzten Diesel Motoren*. PhD thesis, Swiss Federal Institute of Technology (ETH), 1998. Diss. ETH Nr. 12954.