Preprint Cambridge Centre for Computational Chemical Engineering ISSN 1473 – 4273

Multiobjective optimization of a kinetics-based HCCI model using engine data

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released: 12 August 2011

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Preprint No. 106

Keywords: Multiobjective optimization, Stochastic reactor model, HCCI engine

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Abstract

A multi-objective optimization scheme based on stochastic global search is developed and used to examine the performance of an HCCI model containing a reduced chemical kinetic mechanism, and to study interrelations among different model responses. A stochastic reactor model of an HCCI engine is used in this study, and dedicated HCCI engine experiments are performed to provide reference for the optimization. The results revealed conflicting trends among objectives normally used in mechanism optimization, such as ignition delay and engine cylinder pressure history, indicating that a single best combination of optimization variables for these objectives does not exist. This implies that optimizing chemical mechanisms to maintain universal predictivity across such conflicting responses will only yield a predictivity tradeoff. It also implies that careful selection of optimization objectives increases the likelihood of better predictivity for these objectives. This may have a particular importance in those practical applications where a high degree of predictivity for a limited number of responses is needed, but only a reasonable computational expense can be afforded. These insights are utilized here to develop a highly predictive HCCI model of engine cylinder pressure history, and to evaluate the model's ability to predict exhaust emissions. The insight provided by multi-objective optimization on the interplay among different model responses could be of great help for guiding mechanism reduction process and for customizing models based on specific needs.

Contents

1 Introduction

Kinetics-based modeling has become an essential tool in combustion studies and for developing combustion systems and technologies. But due to the high computational expense associated with detailed kinetics modeling, reduced kinetics are favored especially when time and resources are limited or when the modeling aims mainly at evaluating potential alternatives or obtaining a preliminary insight. Kinetic mechanism reduction speeds up computations but inevitably compromises model predictivity. This necessitates the application of an optimization step to guide the reduction process and restore as much predictivity as possible. Approaches for optimizing chemical reaction rates of reduced mechanisms vary from the simple deterministic gradient-based to the more sophisticated stochastic and evolutionary search methods. These latter methods have recently gained wide acceptance and use because of their effectiveness and ability to handle complex search landscapes. Optimization based on evolutionary search is often employed for a single objective [6–8, 11, 12, 14], but there have been also some studies that utilize multiple objectives to enhance the predictivity over a wide range of applications [9, 13].

In general practice, reduced mechanisms are optimized primarily to match experimental ignition delay times. These mechanisms are sometimes also tuned manually to match other responses of interest (i.e. objectives) after a good fit with ignition delay times is established. Some recent studies utilizing multi-objective optimization used flame information in addition to ignition delay times in an attempt to expand the predictivity to combustion systems where flame propagation plays a major role [9].

But as the above approaches focus on optimizing reduced mechanisms to fit mainly ignition delay data, predictivity of actual engine responses is often undermined. This makes such reduced mechanisms of less value for certain practical engine computations. The current work aims specifically at improving predictivity of engine responses of special interest, such as engine cylinder pressure and exhaust emissions. The work employs a multi-objective optimization approach based on evolutionary genetic algorithm, where subsequent search is guided by results from the preceding solutions. Successful solutions from one generation are combined to serve as parents to the population of next generation, with some random changes (i.e. mutations) allowed from time to time in order to explore new regions in the search space and escape the traps of local minima.

As the main objective of the current work is to develop a more predictive model customized for a given engine and a specific modeling setup, the optimization is performed primarily using engine data, and results for ignition delay times are only used for comparison and guidance. In addition, the physical model and the mechanism are treated as one model, and their uncertainties are addressed collectively, rather than individually. Multi-objective optimization is used in this work to study the interrelations among different objectives of interest in order to identify best optimization strategies for achieving targeted enhancement in predictivity.

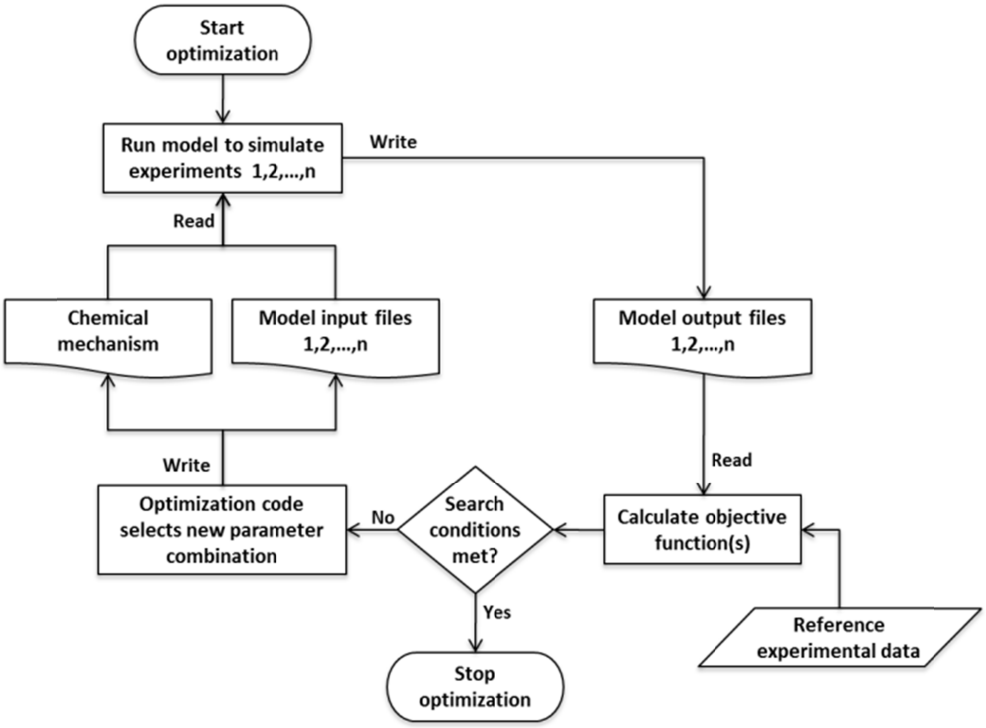

Figure 1: *A flow diagram of the multi-objective genetic algorithm optimization scheme.*

2 Optimization Scheme

Figure 1 shows a flow diagram of the optimization scheme applied in this study. The scheme is built within the MATLAB environment, and uses MATLAB's multi-objective genetic algorithm search function that comes as part of the Global Search toolbox. A stochastic reactor model (SRM) based on probability density function [1–4, 15] is used in the scheme to simulate 12 different experiments simultaneously, and results are written to corresponding output files. The code then reads these output files and calculates objective functions for the selected responses based on reference experimental data. Aiming at minimizing the objective functions, the genetic algorithm selects a new combination of values for the optimization variables and writes it to the input files of the SRM. This cycle is repeated until the optimization termination criteria are met.

The optimization variable set consisted of the three coefficients of Arrhenius equation (i.e. the pre-exponential factor, the temperature exponent and the activation energy) for selected reactions, as well as four variables from the SRM (average wall temperature, residual gas fraction, turbulent mixing time and heat transfer coefficient). Constraints were applied on all variables in the optimization set to preserve the general characteristics of the original model. Variations of Arrhenius coefficients were constrained within $\pm 50\%$ of their original values, while SRM variables were constrained within presumed reasonable ranges.

3 Engine Experiments

The experiments for this work were carried out on a half-liter single-cylinder research engine running in HCCI mode. The specifications of this engine are listed in Table 1. The engine has a pent-roof combustion chamber fitted with four valves. Fuel is delivered intermittently via a port fuel injector located at the end of the intake port just above the intake valves. Intake air passes through a conditioner to adjust its temperature, humidity, and pressure as necessary.

Table 1: *Engine specifications and valve timing information. Crank angles here are measured relative to firing TDC.*

Parameter	**Value**
Number of cylinders	1
Operation cycle	4-stroke
Combustion mode	HCCI
Number of valves	4
Cylinder displacement (liters)	0.5
Bore x Stroke (mm)	84 x 90
Connecting rod length (mm)	159
Crank radius (mm)	45
Compression ratio	12:1
Fuel delivery system	PFI
Cooling water temperature (^{o}C)	90
Lubrication oil temperature (^{o}C)	90
IVO (CAD)	-356
EVC (CAD)	-352
IVC (CAD)	-156
EVO (CAD)	170

The experiments were performed at boosted intake pressure of 1.5 bar and intake air temperature of 75^{o}C. The engine was fueled with primary reference fuels at three different volume ratios: PRF40 (i.e. 40% iso-octane and 60% n-heptane), PRF60 and PRF80. Load sweeps were performed at three constant speeds of 1200, 1500 and 1800 rpm. Upper and lower bounds of possible load range are first identified at each test condition, and then test points are selected at reasonably-distanced intervals. The load range is bounded by knocking and misfire limits, identified in this work respectively by maximum pressure rise rate of 10 bar/deg and CoV in IMEP of 5%.

4 Results

The developed optimization scheme was applied on a reduced chemical kinetic mechanism for primary reference fuels that has 157 species and 1552 reactions. More description of the mechanism can be found in [3, 5]. A temperature sensitivity analysis

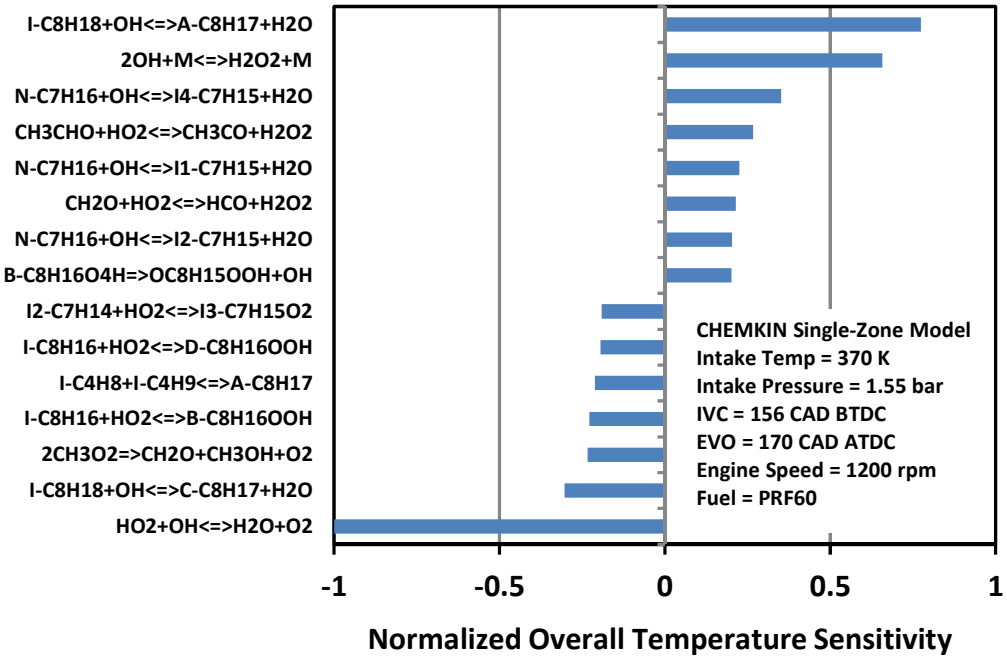

Figure 2: *Normalized temperature sensitivities for the fifteen most dominant reactions in the 157 species PRF mechanism with PRF60 and at engine speed of 1200 rpm and equivalence ratio of 0.3.*

was conducted, using CHEMKIN's single zone HCCI model, to identify the fifteen most dominant reactions in terms of heat release at various engine operating conditions (Figure 2 depicts results for one of these conditions). Arrhenius coefficients for selected reactions along with the selected SRM parameters were then optimized against results from 12 experiments at different operating conditions.

The optimization objectives included cylinder pressure and CO and HC emissions. Objective functions for these responses were formulated in the form of sum of non-weighted squared differences between engine experiment and SRM model values. Five points on the cylinder pressure curve (10^o BTDC, 5^o BTDC, TDC, 10^o ATDC, and 30^o ATDC) were selected to calculate the pressure objective function, and single-point squared differences were used to calculate the CO and HC objective functions.

$$\mathrm{OF}_{\mathrm{pressure}} = \sum_{i=1}^{12}\sum_{j=1}^{5}(P_{\mathrm{sim},i} - P_{\mathrm{exp},i})_j^2 \tag{1}$$

$$\mathrm{OF}_{\mathrm{CO}} = \sum_{i=1}^{12}(CO_{\mathrm{sim},i} - CO_{\mathrm{exp},i})^2 \tag{2}$$

$$\mathrm{OF}_{\mathrm{HC}} = \sum_{i=1}^{12}(HC_{\mathrm{sim},i} - HC_{\mathrm{exp},i})^2 \tag{3}$$

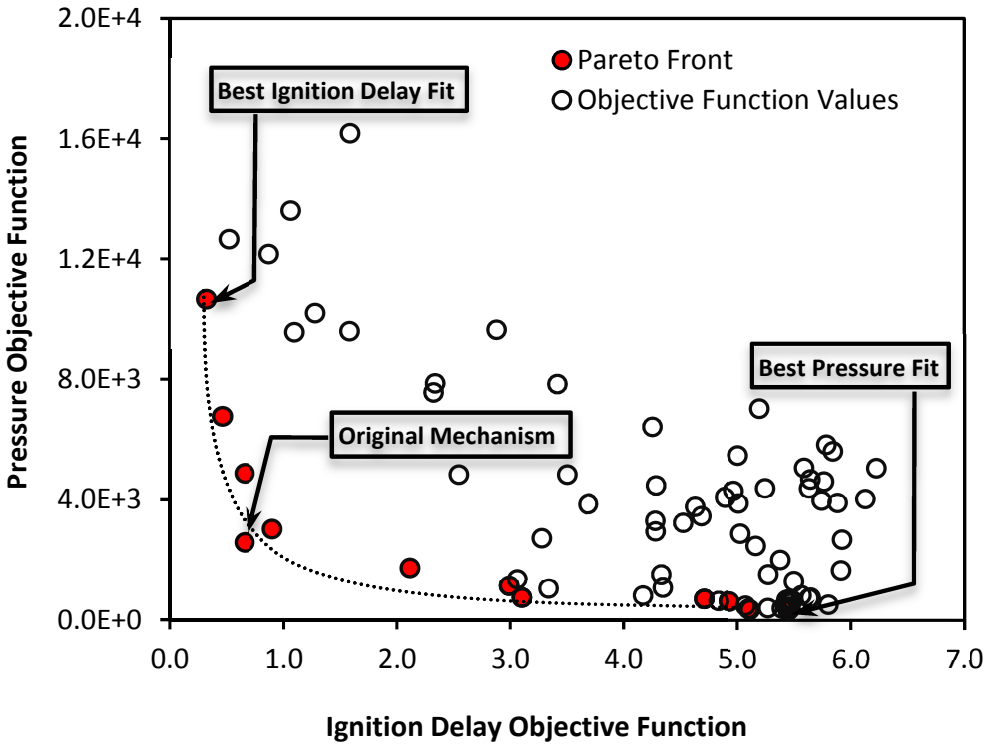

Figure 3: *Solution space and Pareto front for cylinder pressure and ignition delay time objective functions. A clear conflict exists between the two, suggesting that a single best solution for the two cannot be obtained.*

Ignitions delay times corresponding to all solution points were calculated offline using a closed homogeneous batch reactor model in CHEMKIN, and shock tube experimental data from [10] were used for calculating the ignition delay objective function. The calculation was based on nine temperature points on the ignition delay curve, and the objective function, in this case, was formulated in the form of sum of non-weighted squared relative differences, as follows:

$$\mathrm{OF}_{\text{ignition delay}} = \sum_{i=1}^{9} \left(\frac{\tau_{\text{sim},i} - \tau_{\text{exp},i}}{\tau_{\text{exp},i}} \right)^2 \tag{4}$$

This modified formulation takes into account the large difference in ignition delay magnitude at low and high temperatures.

Pressure objective function is plotted against that of the ignition delay in Figure 3, and Pareto front (i.e. the set of optimum solutions) is identified. The plot shows a typical trend for competing objectives, where improvement in predictability of one objective comes, more or less, at the expense of the other.

The original mechanism (i.e. the one with the original set of Arrhenius coefficients) performed quite well, with its solution falling on the obtained Pareto front and in the region where the two objective functions are closest to their minimum, considering all solutions

obtained within the bounds of current optimization. This may indicate that a deliberate effort was made originally to optimize this reduced mechanism so that it provides a tradeoff in predictivity between ignition delay and pressure history.

The results show, however, that significant improvement in pressure predictability can be achieved if the model is optimized solely for pressure objective. This potential is demonstrated in figures 4, 5, and 6 where predicted cylinder pressures for original and optimized models are plotted against experimental data for a wide range of operating conditions. It should be noted that the SRM parameters in the original model, here and later, were optimized for best pressure fit. For both original and optimized models, a fixed residual gas composition, extracted from exhaust gas for an arbitrary but representative operating condition, was used. The initial pressure at IVC was obtained from the experimental data, and the initial temperature was estimated using a GT-Power 1-D gas dynamics model for the test engine. The SRM model calculates the air mass based on initial conditions, and then uses given equivalence ratio to calculate the fuel mass.

The original model generally under-predicted the pressure value, and the optimization has seemingly shifted the model chemistry to a higher temperature regime to compensate for the low reactivity (see Figure 10). While this had a significantly positive impact on pressure predictability, higher reactivity meant shorter ignition delays in general, as can be seen in Figure 7.

Figure 8 shows the solution space and Pareto front for the objective functions of pressure, CO emissions and HC emissions. While the best solution for cylinder pressure also gives the best solution for HC emissions, a clear conflict exists between pressure and HC emissions on one side and CO emissions on the other side. The original model here also gives a compromise between these conflicting responses.

Predictions for CO and HC emissions at 1200 rpm and different PRF and equivalence ratios are shown in Figure 9. The original model significantly over-predicts the CO concentration especially as the equivalence ratio increases. A comparison of temperature histories (Figure 10) indicates that, in order to obtain the best CO fit, the combustion is almost turned off. Optimization for HC emissions has resulted in slight qualitative improvement, but the optimized model continued to significantly under-predict the HC concentration at the high side of equivalence ratio.

5 Conclusion

In this work, the performance of a reduced PRF mechanism for modeling HCCI combustion was examined using a multi-objective optimization approach. The results revealed conflicting trends among objectives normally used in mechanism optimization, such as ignition delay and engine cylinder pressure history, indicating that a single best combination of optimization variables for these objectives does not exist. Therefore, optimizing chemical mechanisms to maintain universal predictivity across such conflicting responses will only yield a predictivity tradeoff. Careful selection of optimization objectives should increase the likelihood of better predictivity for these objectives. This is especially important in practical engine studies where accurate prediction of only a few model responses

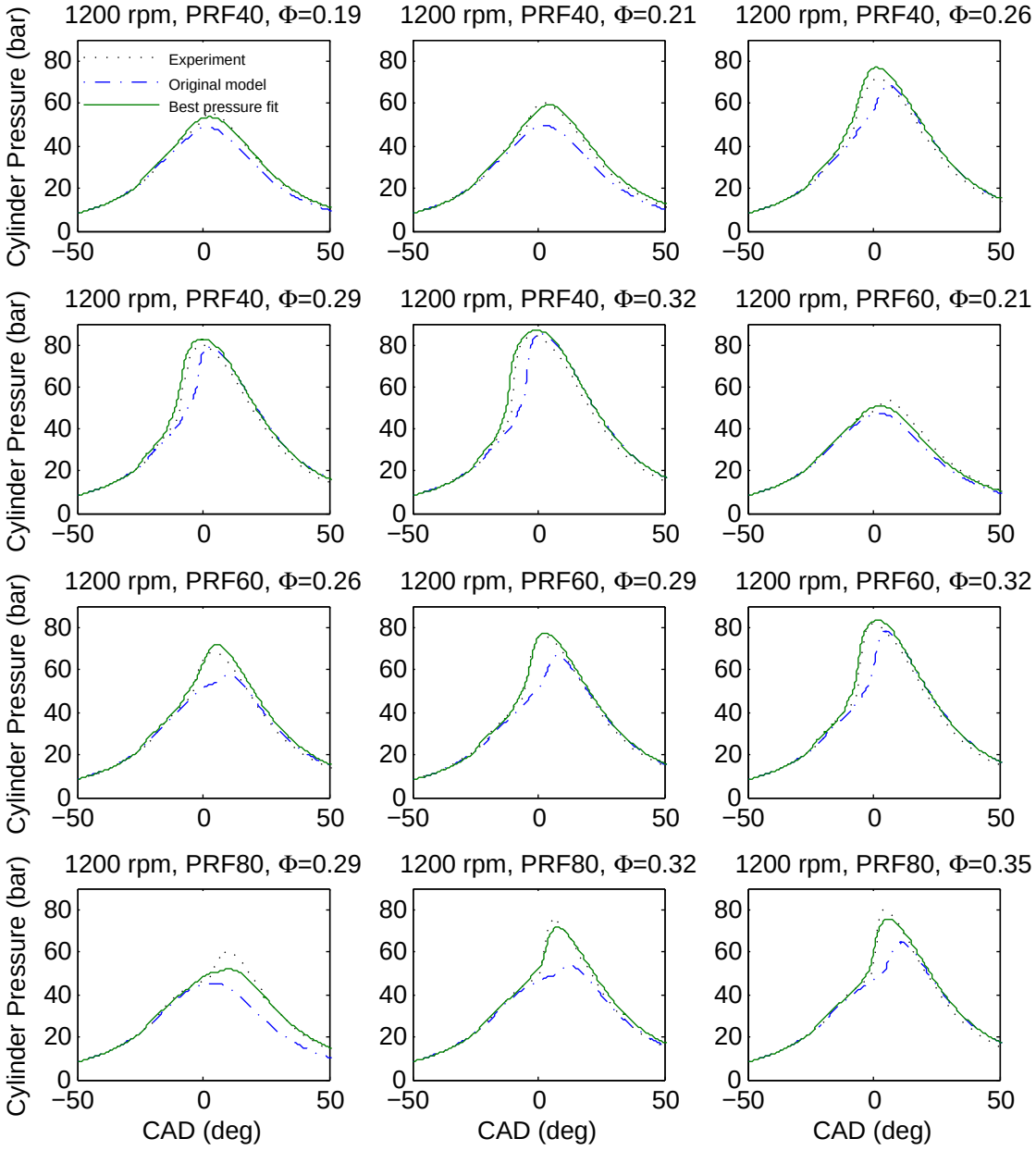

Figure 4: *Comparison of cylinder pressure at1200 rpm and different PRF and equivalence ratios. Improved predictability of cylinder pressure is observed at all conditions relative to the original model.*

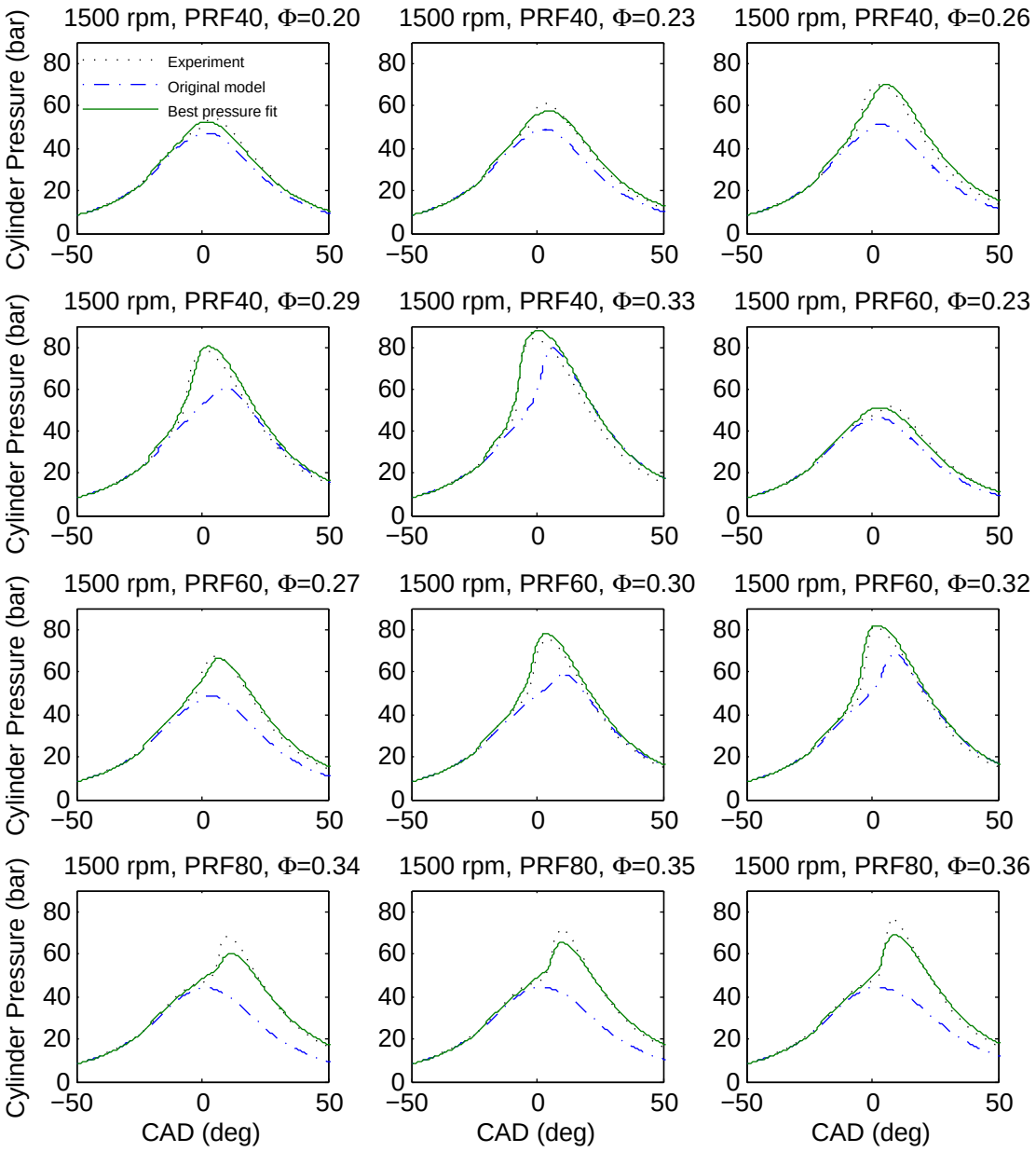

Figure 5: *Comparison of cylinder pressure at 1500 rpm. Here also, the improvement in pressure predictability persists over the whole test range. The original model fails to ignite with PRF80 at 1500 rpm.*

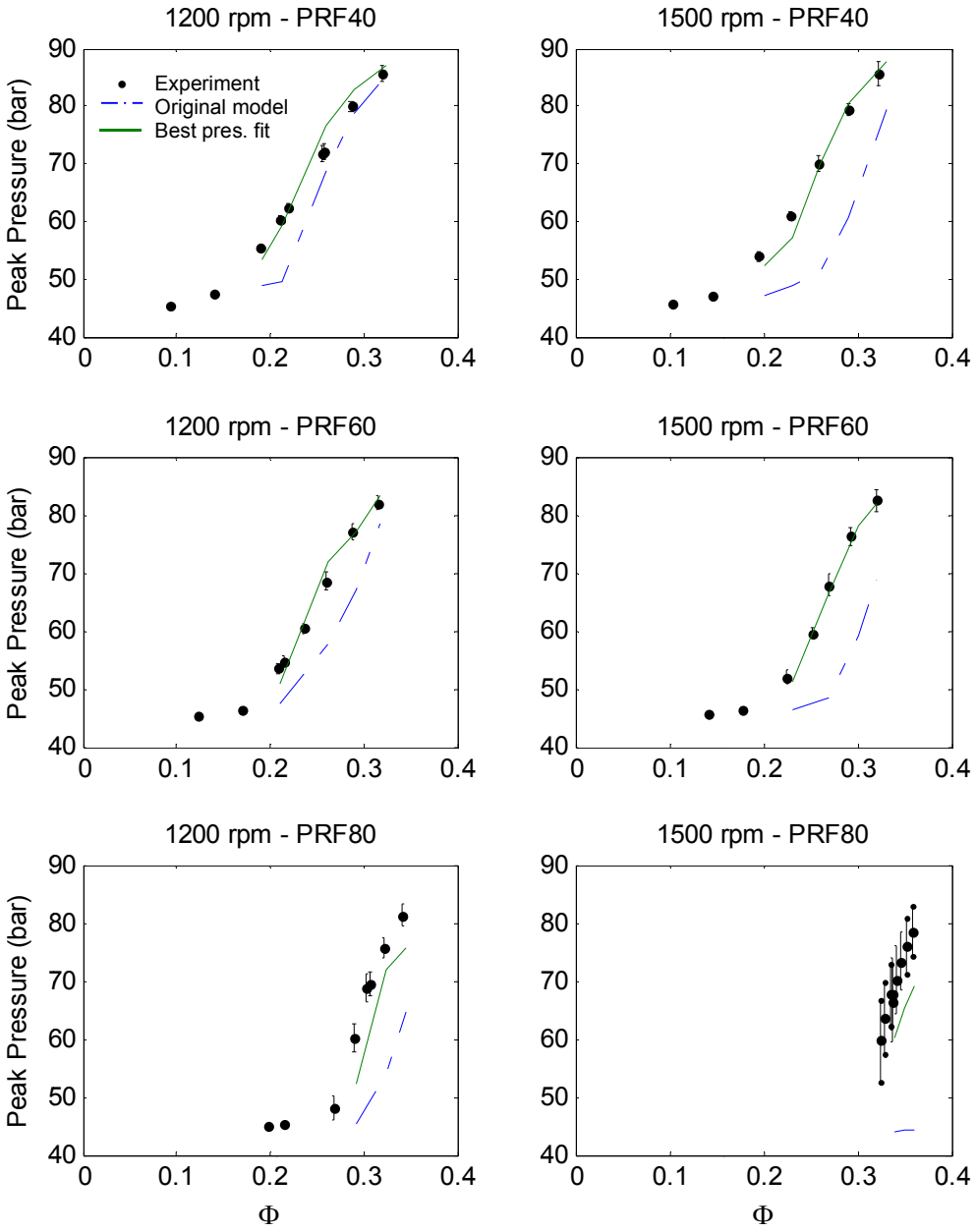

Figure 6: *Improvement in model predictivity of peak pressure for a wide range of operating conditions. Error bars shown on experimental data points are based on one standard deviation. The HCCI operation range is very narrow and quite unstable with PRF80 at 1500 rpm.*

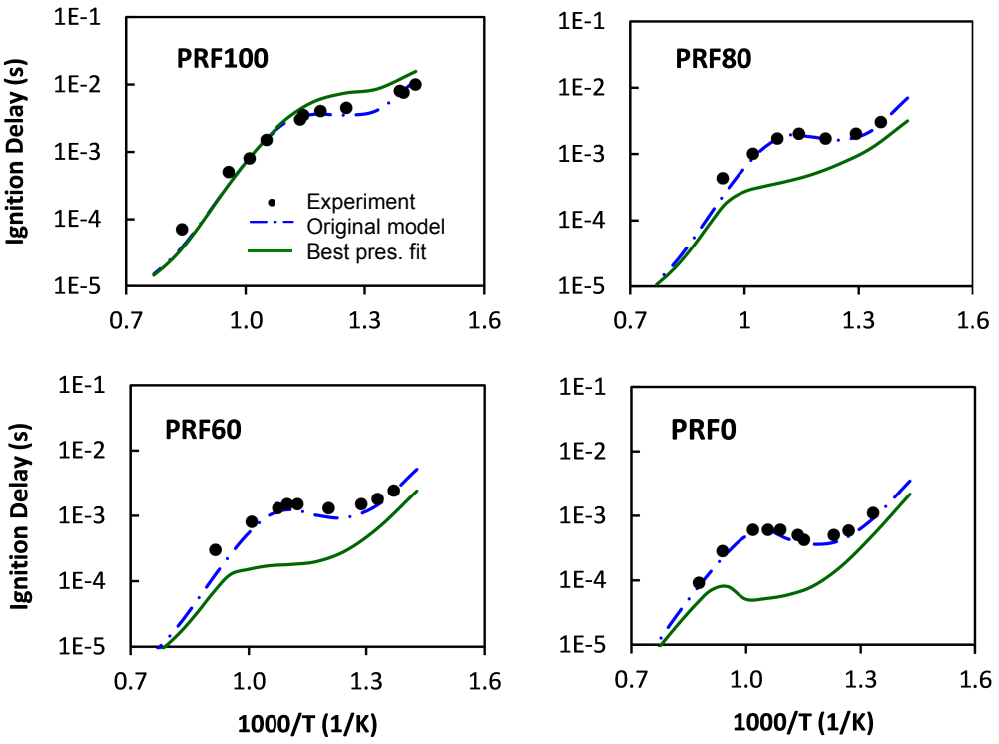

Figure 7: *Ignition delay times with different primary reference fuel ratios, calculated using CHEMKIN's closed homogenous batch reactor model at a pressure of 40 bar and an equivalence ratio of 1.0. Experimental data are taken from [10]. The optimization shifts the model chemistry to a higher temperature regime to compensate for the low reactivity of original mechanism, and this results in shorter ignition delays in general.*

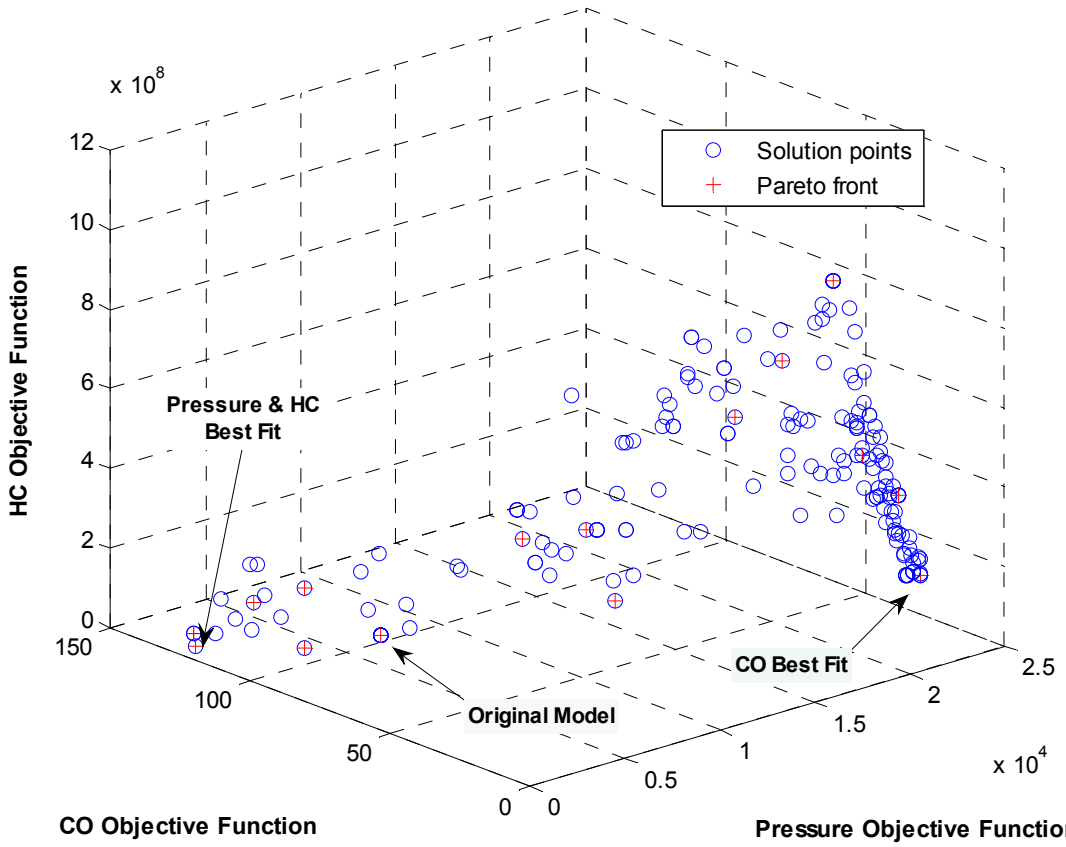

Figure 8: *Solution space and Pareto front for cylinder pressure and CO and HC emissions. The best solution for cylinder pressure gives the best solution for HC emissions, while a clear conflict exists between pressure and HC emissions on one side and CO emissions on the other side, suggesting nonexistence of a single best solution for them.*

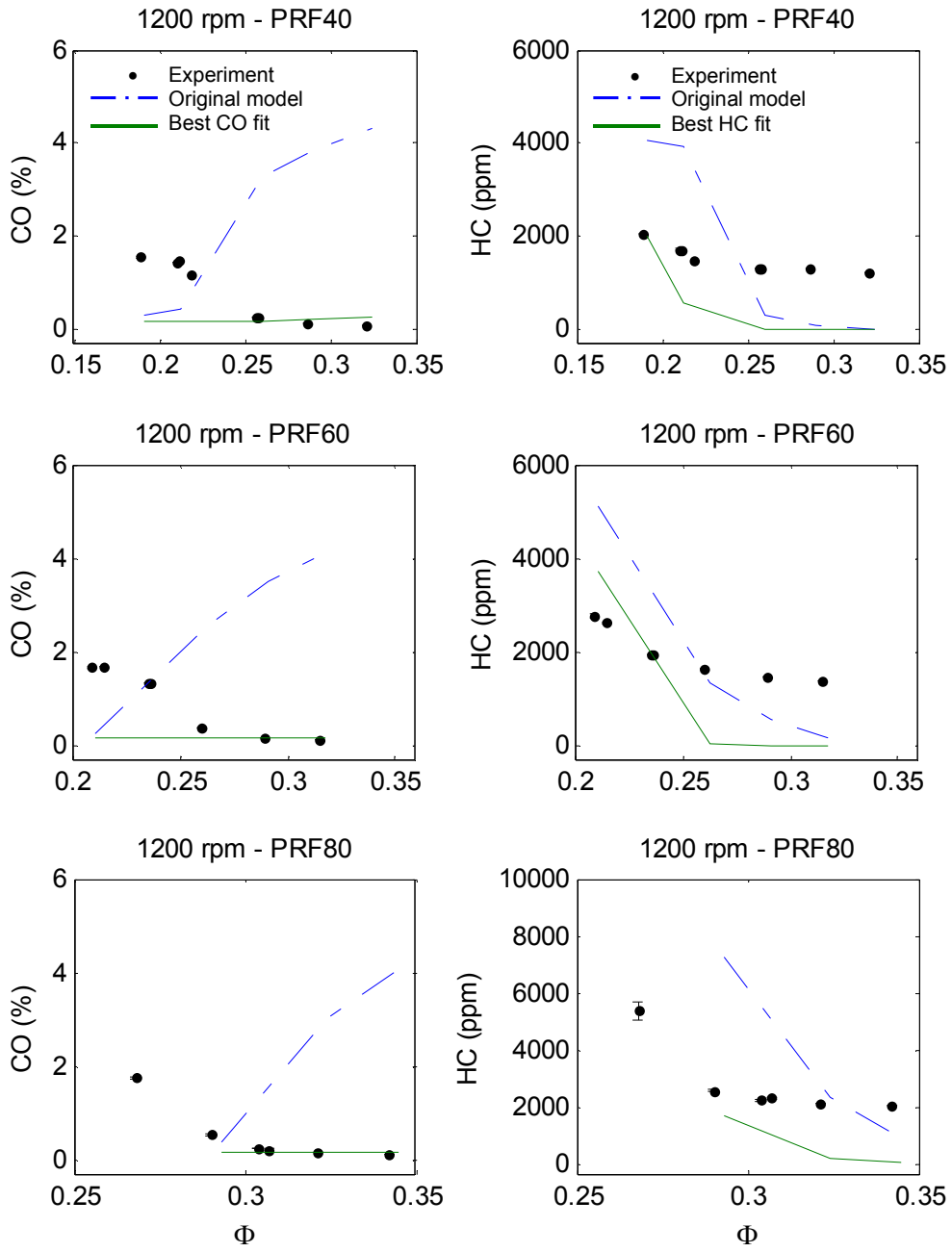

Figure 9: *Predictions for CO and HC emissions at 1200 rpm and different PRF and equivalence ratios. The original model significantly over-predicts the CO concentration especially as the equivalence ratio increases, which makes it difficult to obtain a good fit without shutting off the combustion. Optimization for HC emissions objective has only resulted in slight qualitative improvement.*

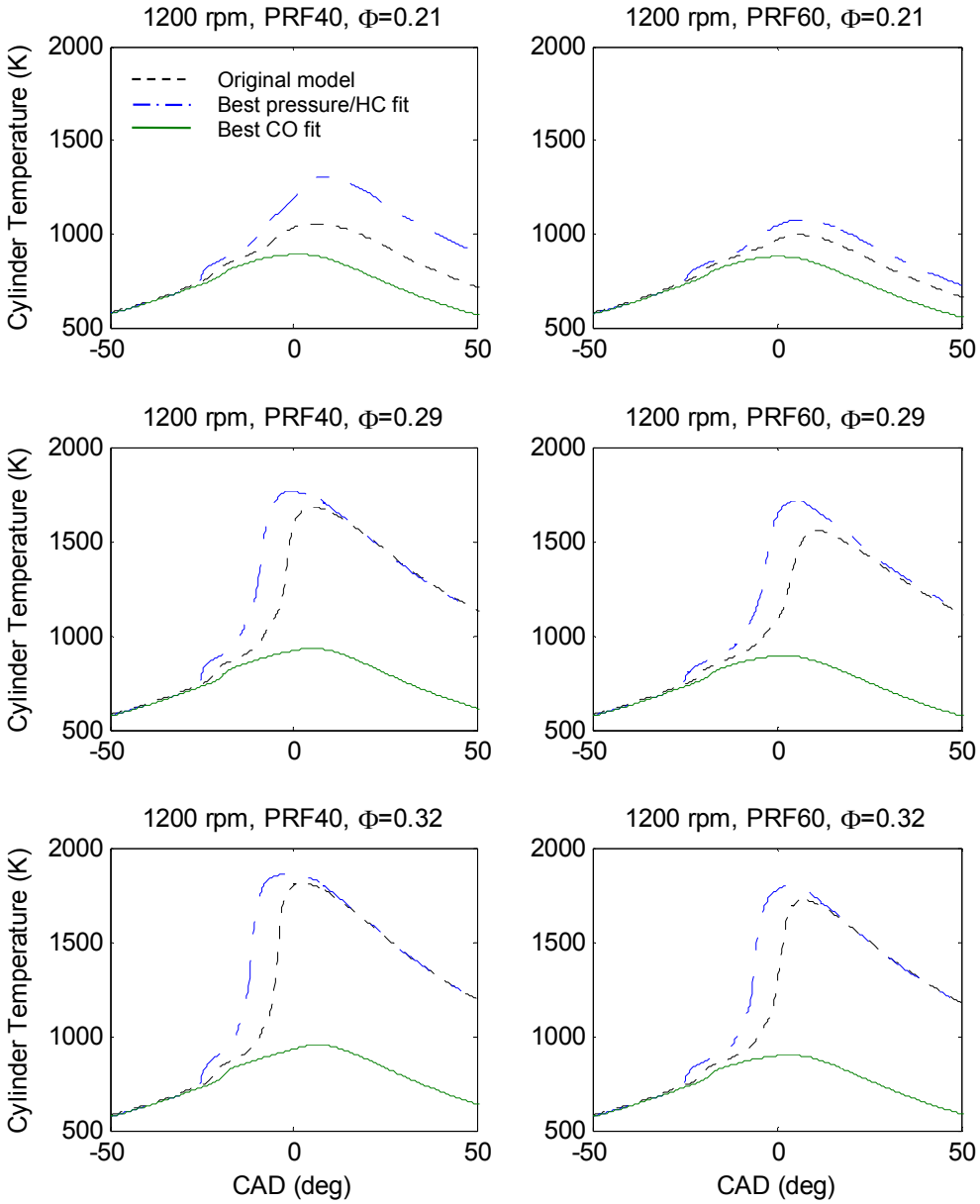

Figure 10: *Cylinder temperature history. Optimization for best pressure increases the reactivity of the mechanism and lifts the chemistry to a higher temperature regime. In contrast, the combustion is almost shut off to obtain the best fit for CO emissions.*

is sought, as it allows for the use of reduced chemistry models while ensuring sufficient predictability of the targeted responses. These conclusions have been demonstrated in this study through development of a highly predictive HCCI model for engine cylinder pressure history, and through improving the model predictivity of engine exhaust emissions.

The use of multi-objective optimization offers more freedom for customizing kinetic models based on intended purpose. One could choose to optimize the kinetic model to give a good compromise among a number of conflicting responses, or to give the best fit for one or two selected responses. The approach, therefore, provides a practical alternative to using computationally expensive detailed kinetic models in those cases where universal predictivity is not required. It also provides useful insight on the goodness of the reduced mechanism and, by exposing the interplay among different model responses, helps in guiding the reduction process to give a better performance. Although the paper presents results for only three engine responses, the approach can be extended to include any response for which experimental results can be obtained.

6 Acknowledgement

The authors would like to thank Yoann Viollet, Marcin Plociniczak and Hassan Babiker of Saudi Aramco's R&D Center for their efforts in carrying out the HCCI engine experiments.

7 Definitions, Acronyms and Abbreviations

ATDC	After top dead centre
BTDC	Before top dead centre
CAD	Crank angle degree
CO	Carbon monoxide
CoV	Coefficient of variation
EVC	Exhaust valve closure
EVO	Exhaust valve opening
HC	Hydrocarbons
HCCI	Homogeneous charge compression ignition
IMEP	Indicated mean effective pressure
IVC	Intake valve closure
IVO	Intake valve opening
PFI	Port fuel injection
PRF	Primary reference fuel
SRM	Stochastic reactor model
TDC	Top dead centre
Φ	Equivalence ratio

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