Optimization of methane-hydrogen blends in a spark-ignition engine using a quasi-dimensional combustion model and genetic algorithm

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Abstract. The objective of the present study is to determine the optimal composition of methane/hydrogen blends in a spark-ignition (SI) engine. First, a quasi-dimensional (QD) model for the simulation of combustion of methane-based fuel blends in SI engines coupled with a chemical kinetics tool for ignition chemistry calculations was developed. Then, the validation was performed by comparing numerical pressure traces against experimental data on a small size single-cylinder engine. Calibration and sensitivity analysis was carried out to assess the predictive capability of the model. Finally, a genetic algorithm (GA) was used to optimize the blend composition and engine input parameters based on a merit function. This methodology resulted in improved indicated thermal efficiency and acceptable level of NOx emissions compared to the baseline design.

Keywords: SI engine; methane-hydrogen; QD model; optimal fuel blend; NO_x emissions

Introduction

Increasing oil prices as well as energy demand per capita and stringent CO_2 emission regulations, motivate the use of alternative fuels in the transport sector [1]. Natural gas (NG) as well as synthetic methane-based fuels have a crucial impact on reducing CO_2 emission from the transportation sector thanks to their favorable H/C ratio. Additionally, the high octane number and high knock resistance of methane allows to run the engine on higher compression ratios [2, 3]. Lean NG combustion has shown the potential to improve efficiency compared to stoichiometric gasoline engines, but suffers from the limited ignitability and unstable combustion of lean NG mixtures [4]. Hydrogen has been considered as a suitable candidate as additve for NG engines [5]. Its higher laminar flame speed, small quenching distance and wider flammability limits can compensate for the demerits of the lean-burn combustion in NG-fueled engines [6, 7]. However, the optimal composition of the fuel blend should be determined to meet requirements of improved efficiency and low exhaust emissions. Using simple models, Paykani et al. [8] studied how conflicting requirements such as maximum ignition delay time and laminar flame speed can be met by adding gaseous components such as hydrogen, syngas or propane to methane to obtain optimal fuel blends under engine-relevant conditions. While simple models were used in that study, that first step investigated the potential of using optimization to determine computationally the optimal composition of gaseous fuels for SI engines using low dimensional models.

Currently, 0D/1D and multi-dimensional engine simulations are being widely used in the engine development process. Quasi-dimensional (QD) models have been developed to bridge the gap between 0D and multi-dimensional models. Having modest computational requirements, QD models can effectively relate the model outputs to the combustion chamber geometry [9]. There are several papers where a QD combustion model has been used, but few were successful to adapt an additional fuel or conduct simulations over different blending ratios due to the change in laminar flame speed [10]. The aim of the present work is to develop a methodology for simultaneous fuel blend and engine input parameters optimization using QD-GA approach in a methane/hydrogen fueled SI engine.

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Research methodology

A predictive two-zone, quasi-dimensional (QD) modeling and genetic algorithm (GA) optimization study are performed to determine the optimal methane/hydrogen fuel blends in SI engines. QD models are known for their predictive expression for the mass burning rate and the inclusion of geometric parameters in the form of a thin, spherical flame front interface separating the burned from the unburned gases [9]. The accuracy of the submodels is crucial for the predictive capability of a QD model. Submodels are needed for closing the equations for pressure, temperatures and masses of the two zones. An ignition submodel is needed for the prediction of flame kernel development, a combustion submodel for computing the mass burning rate and a model of heat transfer through the walls. In addition, a submodel was implemented for the quantitative prediction of NOx emissions. The schematic of the QD model is shown in Fig. 1. Due to the lack of an accurate correlation for the calculation of laminar flame speeds of gaseous fuels blends, reaction kinetics calculation has been carried out using Cantera [11].

A traditional simple genetic algorithm (SGA) approach was used for the problem optimization in Matlab environment [12, 13]. It uses a large population that is evolved through many generations until the optimum is reached. The model variations generated by the SGA are controlled by an objective merit function. A properly defined merit function (MF) is important for the efficiency and success of a GA. In this study, the following merit function is used based on the work of Montgomery [14]:

$$Merit = \frac{1000}{k_1\left(\frac{NO_x}{NO_{x\_Base}}\right)^{n_1} + k_2\left(\frac{\eta_{h\_Base}}{\eta_{th}}\right)^{n_2}}, k_1, n_1 = 2; k_2, n_2 = 1 \quad (1)$$

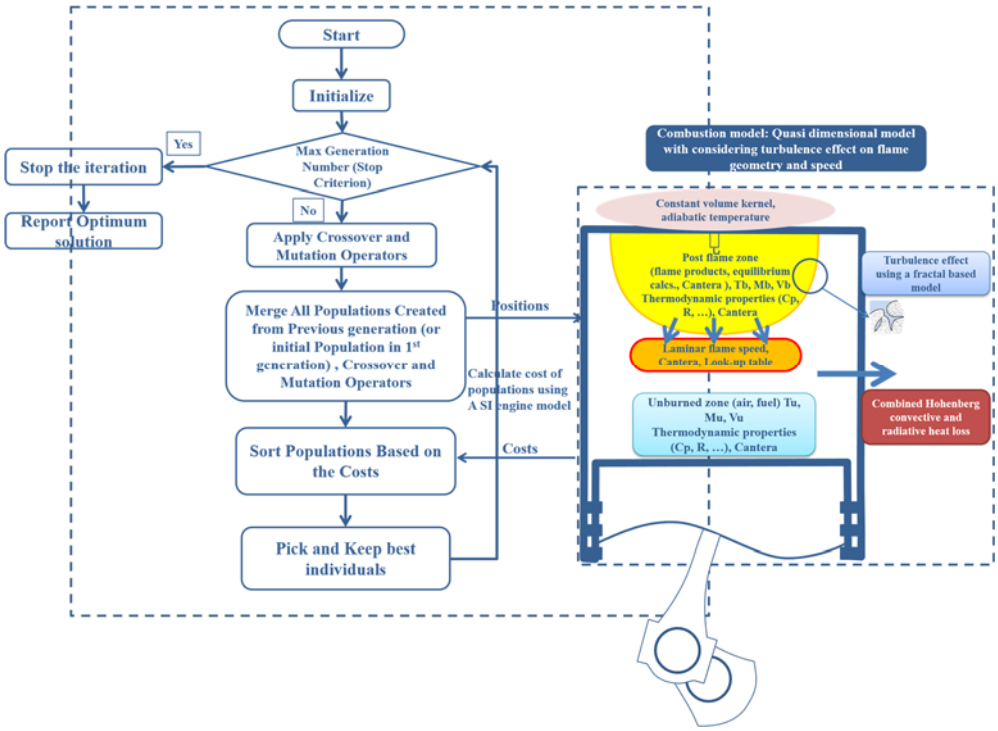


Fig. 1. Flowchart of the research methodology.

The GA was ran with a population of 40 individuals for 50 number of generations. Each individual is a QD simulation case with a set of input parameters. Each generation consists

of a population, which consists of the best individual from the previous generation. The initial population of 40 individuals was generated randomly. The merit values for the individuals were evaluated after each generation is completed and the population is monitored for similarity between the individuals. Convergence was achieved when the GA reached a maximum merit value. The flowchart of the research methodology is illustrated in Fig. 1.

Results and discussion

Model validation

A series of measurements were carried out on a Swissauto Wenko 250cc single cylinder four-stroke spark ignition engine. The experimental data considered in this study consider the effect of methane/hydrogen ratios, air-fuel ratios and spark timings at a constant speed of 3000 rpm. The validation matrix can be seen in Table 1. Model validation focused on calibration of five coefficients affecting the flame development, turbulence–flame interaction and heat transfer submodels in the QD model. For the optimization study, we need a specific set of coefficients, which can yield good in-cylinder pressure predictions for the desired range of the operating conditions. Since it is unlikely to achieve this goal with a single set of coefficients over the full range of interest, a narrow range of operating parameters was selected ($1.4 \le \lambda \le 1.6; 45 \le ST \le 60 CABTDC; 0.0 \le f_{H_2} \le 0.25$). We are currently calibrating the QD model to wider operating ranges and in particular leaner mixtures and higher hydrogen fractions by using different sets of coefficients within different operating windows. The QD model coefficients are calibrated using multi-objective optimization to minimize the root mean square error between measured and calculated in-cylinder pressure by means of GA. Simulation results at different conditions are compared to the experimental in-cylinder pressure traces in Fig. 2, showing a good agreement.

Table 1. Validation cases and operating parameters.

Case	Speed	f_{H_2}	λ	Spark timing (ST)
	(rpm)	(%)	(-)	(CA BTDC)
1	3000	0	1.4	45
2	3000	10	1.4	45
3	3000	25	1.4	45
4	3000	25	1.4	50
5	3000	25	1.4	60

Optimization results

The composition of methane/hydrogen blends and spark timing were optimized for the SI engine operating conditions at fixed $\lambda = 1.4$. The optimization is currently extended to include λ within the aforementioned range where the model was validated. The input parameters and the corresponding outputs for both the base case (case 1 in Table 1) and the optimal case from simulations are listed in Table 2. The optimal case found by QD-GA yielded higher indicated thermal efficiencies (ITE) and slightly increased NOx emissions over the baseline design. Fig. 3(a) presents ITE versus NO_X emissions points for this optimization study obtained from 2000 simulations. The temporal evolution of in-cylinder pressure for both the base and optimal cases are shown in Fig. 3(b). Clearly, the total work done in the optimal case is higher, thereby resulting in higher ITE. Hydrogen addition increases combustion and thermal efficiencies due to shorter burn duration. The NOx emissions are higher in the optimal case because of the higher combustion temperatures

associated with hydrogen addition. The increased laminar flame speed obtained from addition of hydrogen results in faster combustion and therefore higher temperatures inside the cylinder, which leads to higher NOx emissions at constant λ [15].

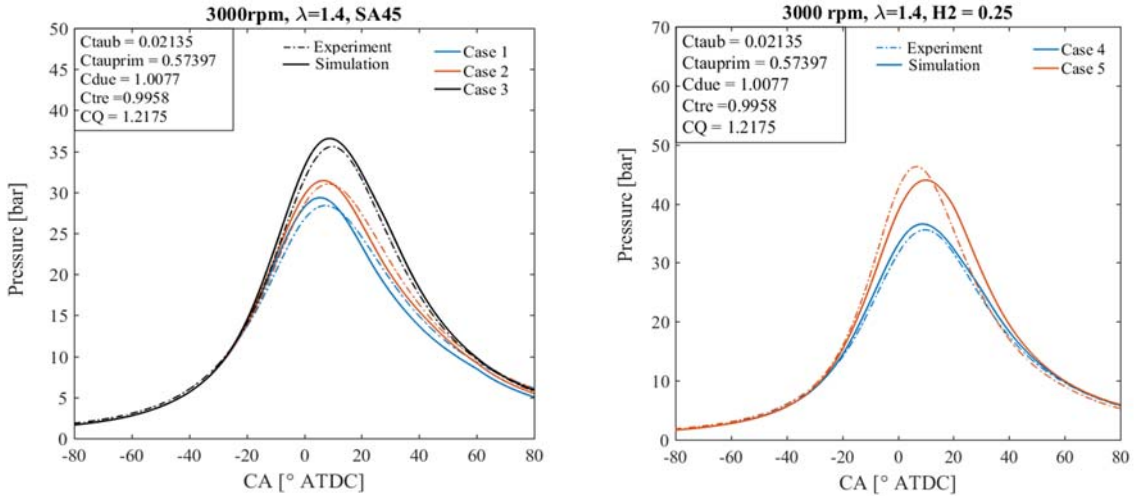
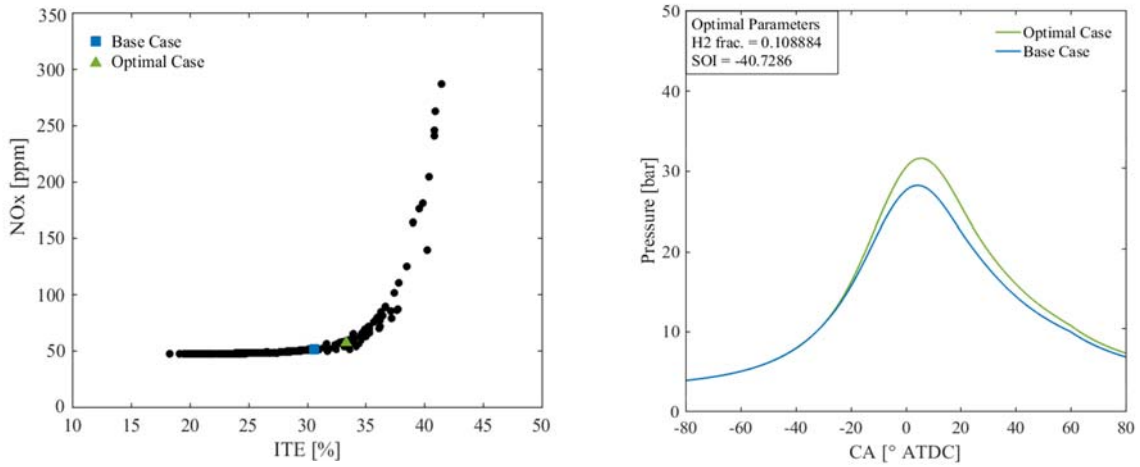


Fig. 2. In-cylinder pressure validation and coefficients calibration for different cases.



(a) (b)

Fig. 3. (a) ITE versus NOx for all simulation cases including the base and optimum; (b) Temporal evolution of in-cylinder pressure for base and QD-GA optimal cases.

Conclusions

A QD-GA methodology is implemented to compute the optimal fuel composition and spark timing based which maximize the indicated thermal efficiency and minimize NOx emissions for a high speed SI engine for which baseline engine experimental data is available. It was found that the present methodology could reach an optimal design with favorable indicated thermal efficiencies and at the cost of modestly higher Ox emissions compared to the baseline case. The lean limit extension with higher H_2 amounts allows for operation at higher λ, where the NOx-ITE tradeoff can be shifted towards NOx emissions below the base values.

Table 2. Input parameters and outputs for the baseline and QD-GA optimal cases.

Parameter	Base case	Optimal case
Inputs		
Fuel composition (%vol)	100% CH_4	89.12%CH_4/10.88%H_2
Air-fuel ratio (λ)	1.4	1.4
Spark timing (CA BTDC)	45	40.72
Outputs		
ITE (%)	31.4	33.9
NO_x (ppm)	49.8	62.7

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