Optimization of composition of methane/syngas mixtures at engine-relevant conditions: A NSGA-II coupled TOPSIS approach

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Abstract

The addition of syngas to methane can enhance combustion quality at low loads in natural gas internal combustion engines (ICEs), however the optimal composition of syngas in the mixture should be determined to meet requirements of a high-quality combustion. In this paper, a coupled evolutionary optimization approach integrating a non-dominated sorting genetic algorithm (NSGA-II) and a technique for order preference by similarity to ideal solution (TOPSIS) is employed to find the optimal methane/syngas composition at conditions relevant for spark ignition (SI) engines. The objective is the simultaneous minimization of the ignition delay time (IDT), and the maximization of laminar flame speed (LFS), and Wobbe number (WN) or Wobbe index (WI). From the obtained set of Pareto solutions, the best compromise solutions are determined by the TOPSIS method. The optimal mixture compositions that could serve as a suitable candidate for satisfying minimum IDT, and maximum LFS and WN are obtained.

Keywords: methane; syngas; optimal composition; NSGA-II; TOPSIS

Introduction

Natural gas (methane as dominating component) is a promising clean alternative fuel to conventional liquid fuels for use in industrial gas turbines and automotive engines due to its availability, high H/C ratio, high octane number and very low particulate matter (PM) emissions. However, it also has some unfavorable combustion characteristics, such as low flame propagation speed at lean conditions [1, 2]. Syngas (which is mainly composed of H_2 and CO) is a suitable candidate for application as a secondary fuel in ICEs. Its high laminar flame speed, small quenching distance and wider flammability limit compensate for the limited lean-burn ability and slow burning velocity of the natural gas [3]. The ignition delay time (IDT) is a key property usually used for validation to provide chemical time scale information for the improvement of chemical kinetics models [4]. The laminar flame speed (LFS) is also a measure of mixture diffusivity, reaction kinetics, and heat release rate, and a key parameter for turbulent combustion [5]. The Wobbe number (WN) is frequently used to compare the combustion energy output of different compositions of fuel gases [2]. It can be calculated by dividing the heating value of gaseous fuel to the square root of its specific gravity.

Evolutionary algorithms are widely used for multi-objective optimization (MOO) of engine performance and emissions because of their natural properties suited for these types of problems. The NSGA-II is a Pareto-based efficient algorithm proposed by Deb et al. [6] for the solution of MOOs. It generates a set of Pareto solutions, where each of them performs better than the rest on at least one criterion. After finding the Pareto solutions, it is desired to find some trade-off optimal points of the objective functions. For this purpose, TOPSIS can be used, a multiple-attribute decision-making (MADM) algorithm that is based on the simultaneous minimization of the distance from an ideal point and the maximization of the distance from a nadir point [7]. Several published research works used NSGA-II to determine the Pareto set and TOPSIS to find the best compromise solutions for different scenarios in optimization stud-

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ies of ICEs [8-10]. In the present work, the composition of methane/syngas mixtures is optimized for high-pressure, lean-burn natural gas-fueled SI engine-relevant conditions using a coupled NSGA-II and TOPSIS approach. The optimal mixture compositions that could serve as a suitable candidate for satisfying the minimum IDT, maximum LFS, and maximum WN are obtained.

Modeling approach

In this work, the GRI-3.0 reaction mechanism is used to model methane/syngas combustion [11]. Simulations of IDT, LFS and WN are performed using the CANTERA reactive flow open source code [12]. IDT is computed based on the maximum of the OH concentration, and LFS is simulated using the FreeFlame class included in CANTERA. The simulations are performed at temperature of 1000 K, pressure of 40 bar and equivalence ratio φ=0.5, which is a typical SI engine operating condition. The NSGA-II is utilized to find the Pareto front through an evolutionary computation procedure. Then, TOPSIS is applied to obtain the best compromise solution, which is the closest to the ideal solution and the farthest from the non-ideal solution of the Pareto set according to the decision maker's objective weights. A convergence metric of the optimization process is defined in order to better monitor the optimization process by averaging the normalized distance for all Pareto solutions of the current generation [13]. A population of 50 individuals with a crossover probability of 0.9 and mutation probability of 0.02 is used in 100 generations for the three-objective optimization problem. The mole fractions of the fuel components are constrained as in the ranges $0.5 \le CH_4 \le 1.0$, $0 \le H_2 \le 0.25$, $0 \le CO \le 0.25$. Another constraint is imposed to ensure that the sum of the mole fractions is unity.

Results and discussion

Comparisons of IDT and LFS for methane/syngas mixtures using different detailed reaction mechanisms are shown in Fig. 1 and 2, respectively, in order to validate the chemical kinetic simulation. It can be seen that there is a good agreement between the simulation and experimental results at low temperatures and lean conditions with the GRI-3.0 mechanism. The obtained Pareto front and the corresponding configuration of optimal methane/syngas mixtures (50 mixture compositions) are illustrated in Fig 3. The different weights considered as reported in Table 1, together with the optimal compositions of methane/syngas mixtures for each weight vector, and are also highlighted in Fig. 3. The configuration plot shows the maximum and minimum limits of the three species. It can be seen that very high CH_4 contents (>95%) corresponds to very low H_2 and CO fractions and vice versa. The majority of optimal points are distributed in the ranges $0.5 \le CH_4 \le 0.8$, $0.2 \le H_2 \le 0.3$, $0 \le CO \le 0.05$. Without any preference for the objective functions, mixtures with high CH_4 and H_2 contents and very low CO are more favorable. It is interesting to note that when LFS or IDT are of high importance, the optimal mixture composition is identical and corresponds to low CH_4 and high H_2 and CO content in the mixture, since H_2 has higher LFS and CO is more reactive than other two components. In addition, since methane has higher WN, TOPSIS chooses a higher amount of CH_4 with low H_2 and negligible CO for the solution when the weight factor for the WN is high (see Table 1).

Conclusions

A kinetic modeling and optimization study was performed to obtain optimal methane/syngas mixture compositions at SI engine-relevant condition. NSGA-II was used to solve a three-objective optimization (i.e., IDT, LFS and WN) problem to find the Pareto front and the corresponding optimal compositions. The decision making TOPSIS method was applied to determine the best compromise solution from the Pareto solutions with different preferences. It was found that minimum IDT and maximum LFS correspond to the mixture with lower CH_4 and higher H_2 and CO percentages. Alternatively, the best composition for maximizing WN corresponds to the mixture with higher CH_4 content (i.e., 92%). The mixture with a moderate content of CH_4 and H_2 and very low CO provided the best compromise solution if no preference for objective functions was considered.

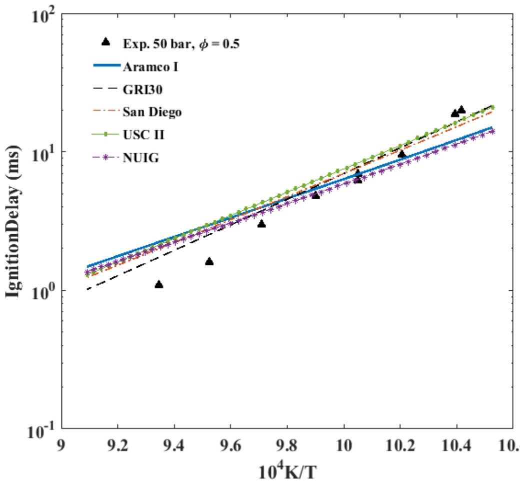

Fig. 1 Comparison of IDT for 50%CH4/30%H2/20%CO at p=50 bar, φ=0.5 for different mechanisms; Symbol represent experimental data [14]

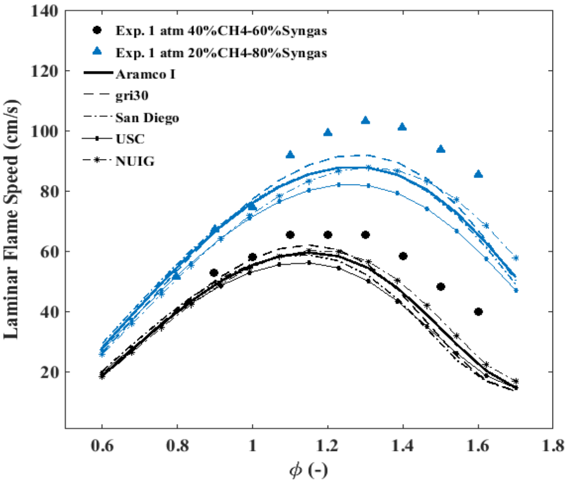

Fig. 2 LFS of $CH_4/H_2/CO$ mixtures at 1 atm as a function of equivalence ratio, T_{ini} = 295 K. Symbols represent experimental data [15]

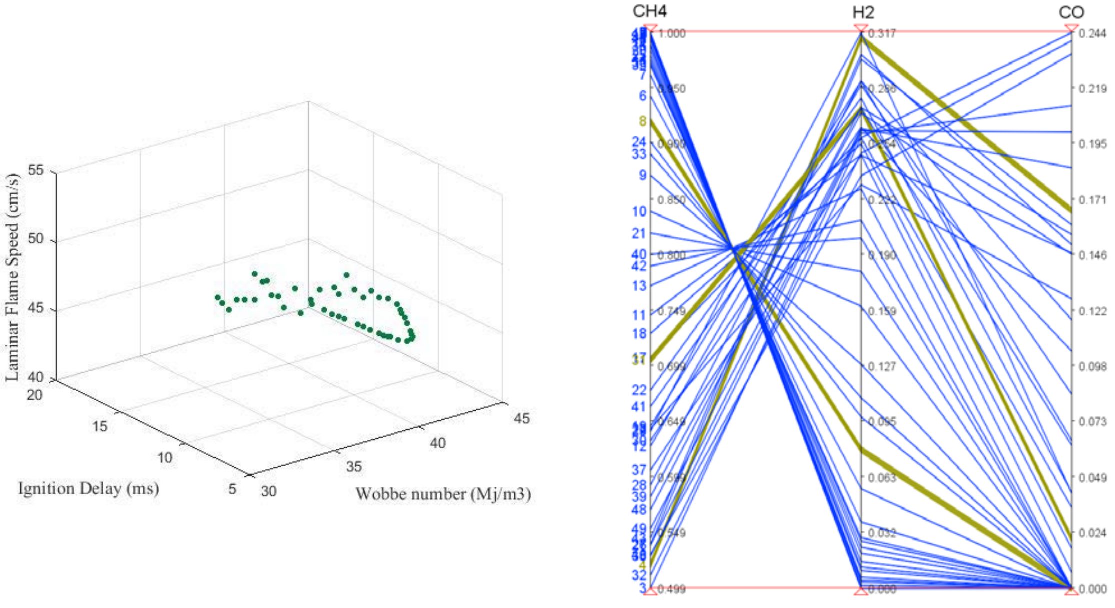

Fig. 3 Parallel chart of optimal methane/syngas mixture compositions found by optimization (the thick lines show the TOPSIS results)

Table 1. Optimal compositions and objective functions according to weight vector

Weight factors (IDT, WN, LFS)	Objective function (IDT, WN, LFS)	Optimal composition (CH_4,H_2,CO)
(0.333,0.333,0.333)	(9.185, 40.426, 47.775)	(0.705, 0.274, 0.022)
(0.8,0.1,0.1)	(8.218, 32.753, 52.116)	(0.520, 0.314, 0.166)
(0.1,0.8,0.1)	(10.637, 43.893, 42.387)	(0.9205, 0.079, 1e-4)
(0.1,0.1,0.8)	(8.218, 32.753, 52.116)	(0.5200, 0.3146, 0.166)

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References

[1] Korakianitis T, Namasivayam A, Crookes R. Natural-gas fueled spark-ignition (SI) and compression-ignition (CI) engine performance and emissions. Progress in Energy and Combustion Science. 2011; 37:89-112.

[2] Kakaee A-H, Paykani A, Ghajar M. The influence of fuel composition on the combustion and emission characteristics of natural gas fueled engines. Renewable and Sustainable Energy Reviews. 2014; 38:64-78.

[3] Lieuwen T, Yang V, Yetter R. Synthesis gas combustion. Fundamentals and Applications. 2010.

[4] Petersen EL, Hall JM, Smith SD, de Vries J, Amadio AR, Crofton MW. Ignition of lean methane-based fuel blends at gas turbine pressures. Journal of Engineering for Gas Turbines and Power. 2007; 129:937-44.

[5] Ranzi E, Frassoldati A, Grana R, Cuoci A, Faravelli T, Kelley A, et al. Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels. Progress in Energy and Combustion Science. 2012; 38:468-501.

[6] Deb K, Pratap A, Agarwal S, Meyarivan T. A fast and elitist multi-objective genetic algorithm: NSGA-II. IEEE transactions on evolutionary computation. 2002; 6:182-97.

[7] Hwang C-L, Yoon K. Multiple attribute decision making: methods and applications a state-of-the-art survey: Springer Science & Business Media; 2012.

[8] Etghani MM, Shojaeefard MH, Khalkhali A, Akbari M. A hybrid method of modified NSGA-II and TOPSIS to optimize performance and emissions of a diesel engine using biodiesel. Applied Thermal Engineering. 2013; 59:309-15.

[9] Kakaee A-H, Rahnama P, Paykani A, Mashadi B. Combining artificial neural network and multi-objective optimization to reduce a heavy-duty diesel engine emissions and fuel consumption. Journal of Central South University. 2015; 22:4235-45.

[10] Deb M, Debbarma B, Majumder A, Banerjee R. Performance–emission optimization of a diesel-hydrogen dual fuel operation: A NSGA II coupled TOPSIS MADM approach. Energy. 2016; 117:281-90.

[11] Smith GP, Golden DM, Frenklach M, Moriarty NW, Eiteneer B, Goldenberg M, et al. GRI 3.0 Mechanism. Gas Research Institute (http://www me berkeley edu/gri_mech). 1999.

[12] Goodwin DG, Moffat HK, Speth RL. Cantera: An Object-oriented Software Toolkit for Chemical Kinetics. Thermodynamics, and Transport Processes. 2015.

[13] Shi Y, Ge H-W, Reitz RD. Computational optimization of internal combustion engines: Springer Science & Business Media; 2011.

[14] Gersen S, Darmeveil H, Levinsky H. The effects of CO addition on the autoignition of H_2, CH_4 and CH_4/H_2 fuels at high pressure in an RCM. Combustion and Flame. 2012; 159:3472-5.

[15] Lapalme D, Seers P. Influence of CO_2, CH_4, and initial temperature on H_2/CO laminar flame speed. International Journal of Hydrogen Energy. 2014; 39:3477-86.