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Heat Transfer effects on Auto-Ignition behavior of Natural Gas and Heptane Fueled HCCI combustion: a Multi-Zone Simulation

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Abstract

The Homogenous Charge Compression Ignition (HCCI) combustion in an natural gas (Methane) and Heptane fueled engine using detailed chemical kinetics is investigated in this research. Sensitivity analysis of O, H, CH and OH species have been performed for the two sample fuels. The effect of heat transfer of start of combustion (SOC) and temperature gradient have been investigated. The SOC shifts to the higher crank angles as the heat transfer is considered because of the heat loss to the cylinder body and later combustion is happening inside the cylinder.

Keywords: HCCI Combustion, Natural Gas, Heptane, Heat Transfer, Detailed Chemical Kinetics

1. Introduction

Very low NO_x and almost no soot emissions and elevated thermodynamic efficiency, made Homogenous Charge Compression Ignition (HCCI) combustion a great candidate combustion methods for next generations of internal combustion engines [1, 2, 3, 4, 5, 6, 7]. The most benefits of HCCI combustion is because of its premixed and lean fast combustion. Large heat release rate (HRR) with a combustion without a flame front [8]. The high thermal efficiency of HCCI combustion is due to its ability to design for high compression ratios (CR), lean and almost constant volume combustion with no throttle loss, [9, 10].

10 There are some obstacles need to be overcome to commercialize the HCCI

engines with these great features. Difficulties in cold start and high HC and CO emissions, and small range of normal operating for HCCI engines are some of the difficulties [11, 12]. One of the challenges for HCCI engine design is controlling the start of ignition for different speed and operational load operating conditions
15 of the engine [13]. So, simulations based on parametric study to approach a reliable control method of HCCI combustion currently is highly demanding by the scientists and engineers[14, 15]. Some examples of methods used to control HCCI combustion, are inlet pressure and temperature changes and altering the compression ratio (VVT method) [16, 17].

20 In order to design an engine which uses HCCI combustion and is reliable for use, controlling is vital to understand the effects of altering each engine and combustion parameter change on HCCI combustion output and behavior. For this purpose, in this research we have performed a study to investigate effects of altering each parameter on HCCI engine combustion to understand effect of
25 inlet pressure, inlet temperature, air fuel ratio, cylinder compression, and engine speed on in-cylinder pressure history, start of combustion of a Natural Gas and Heptane fueled HCCI combustion engines.

2. Methodology

As shown in Fig. 1, the cylinder is divided to five different zones with dif-
30 ferent sizes and shapes; Center volume is centered in the cylinder inside charge, which is an inner gas with a shape of another cylinder which is surrounded by an outer zones with concentric shell of gas. The thickness of these shells are t_1 . The outer zones are cylindrically shaped. The boundary layer is modeled in our simulations too, for this purpose, it is assumed that every zone becomes
35 thinner as we go further from the center towards cylinder walls and the value of R shows the fraction of the thickness of the next layer in comparison to the previous one. Values of the center zone volume is 0.3 of total volume of cylinder.

To model detailed chemical kinetics, we have used the GRI-mech 3.0 chemical kinetic mechanism [18].

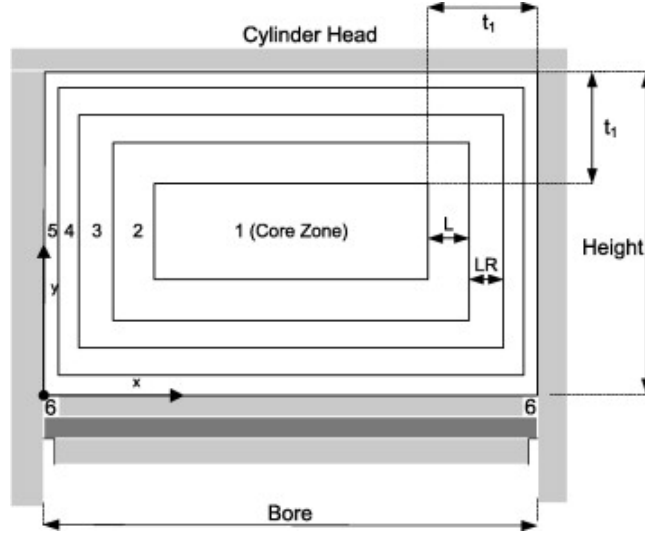


Figure 1: Zone configuration of MZCM.

3. Governing equations

Thermodynamic properties in zones are uniform and it is assumed that the gas is an ideal gas. We also assumed that the mass inside the cylinder is homogenous at the beginning of the simulation. After that point, mass transfer model between zones is happening to keep the in-cylinder pressure uniform for the combustion chamber:

$$\frac{dm_k}{dt} \neq 0 \quad (1)$$

$$\sum_{k=1}^{N_z} m_k = m_{tot} \quad (2)$$

Energy conservation equation is as follows:

$$m_k \bar{c}_v^k \frac{dT_k}{dt} = -m_k \sum_{i=1}^{N_s} U_i \frac{dY_{i,k}}{dt} - P \frac{dV_k}{dt} + \frac{dQ_k}{dt} + m_{i-1 \rightarrow i} h_{i-1} - m_{i \rightarrow i+1} h_i \quad (3)$$

The net rate of species production can be calculated using:

$$\frac{dY_{i,k}}{dt} = \frac{\dot{\omega}_{i,k} MW_i}{\rho_k} \quad (4)$$

Woschnis correlation [21] is used to simulate thermal transport between zones with changes which for HCCI engines and combustion simulations applications [19]. It is used for convective thermal transport modeling inside the cylinder to transfer heat to cylinder wall.

$$h_c(t) = \beta \times Height(t)^{-0.2} P(t)^{0.8} T(t)^{-0.73} \nu(t)^{0.8} \quad (5)$$

Thermal transport among different zones are modeled by a mechanism which is like conduction. So, heat flux of thermal transport will be dependent on the temperature difference of the zones which are neighbor and on the distance as follows:

$$\dot{q} = -K_{tot} \frac{dT}{dy} \quad (6)$$

In Eq. 6, the K_{tot} is a conductivity of total flow which is found by Yang and Martin method [20] and is the summation the turbulent and laminar component.

$$k_{tot} = K_l + K_t \quad (7)$$

The ratio of turbulent to laminar component is calculated by the following equation:

$$\frac{K_t}{K_l} = \frac{Pr_l \mu_t}{Pr_t \mu_l} \quad (8)$$

Eq. 8 presupposes flows. The viscosity ratio can be calculated by:

$$\frac{\mu_t}{\mu_l} = ky_n^+ [1 - \exp(-2\alpha ky_n^+)] \quad (9)$$

and

$$y_n^+ = \frac{u^*}{\mu_w} \int_0^u \rho dy_n \quad (10)$$

here $k = 0.44$ which is the Von Karman Constant, $\alpha = 0.08$ and y_n^+ is the distance between the zone center and the wall. The velocity is proportional to engine rpm.

65 **4. Results and Discussion**

For sensitivity analysis when the mixture temperature has increased by 100 K, 200 K, and 300K, first corresponding time for 1600K, 1700K and 1800K are obtained:

Table 1: Sensitivity analysis of the mixture

Time(s)	T (K)
1.10E-03	1.61E+03
1.10E-03	1.61E+03
1.11E-03	1.62E+03
1.12E-03	1.63E+03
1.12E-03	1.65E+03
1.13E-03	1.67E+03
1.14E-03	1.70E+03
1.15E-03	1.73E+03
1.15E-03	1.75E+03
1.15E-03	1.77E+03
1.16E-03	1.80E+03

At time 0.001099 s corresponding to 1600 K the results of sensitivity analysis
 70 for O, H, CH and OH are as follow:

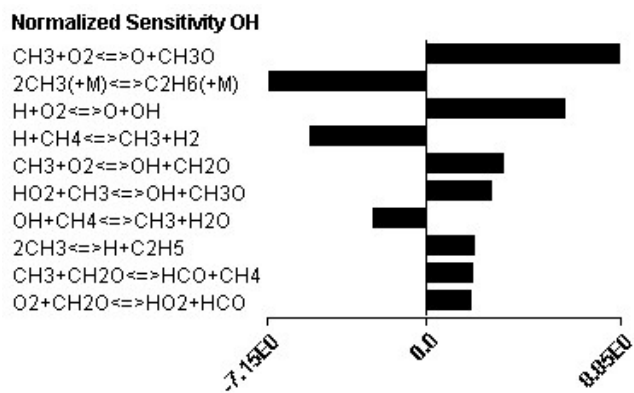


Figure 2: Sensitivity analysis of O.

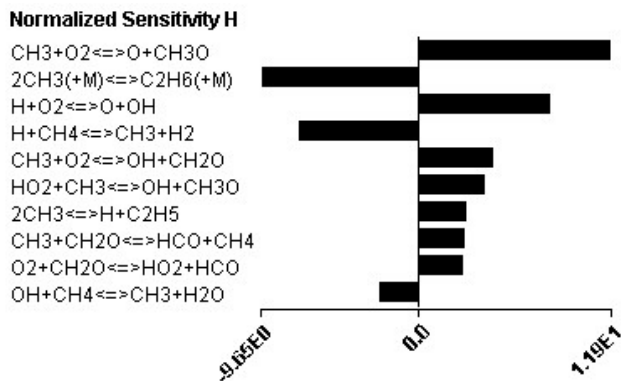


Figure 3: Sensitivity analysis of H.

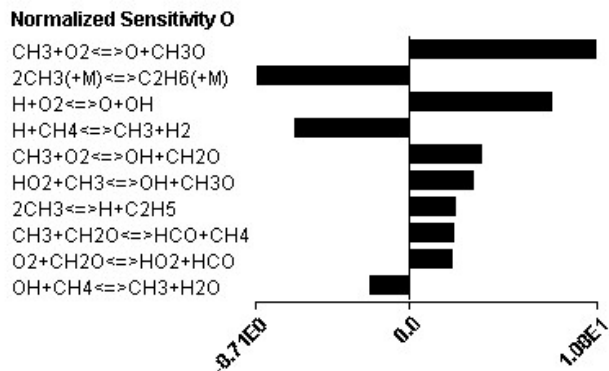


Figure 4: Sensitivity analysis of CH.

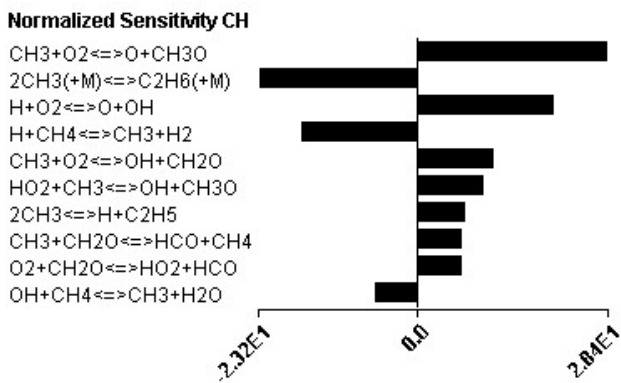


Figure 5: Sensitivity analysis of OH.

At time 0.00114 s corresponding to 1700 K the results of sensitivity analysis for O, H, CH and OH are as follow:

Normalized Sensitivity OH

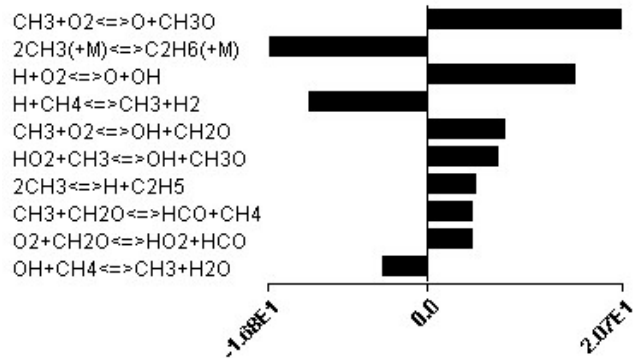


Figure 6: Sensitivity analysis of O.

Normalized Sensitivity H

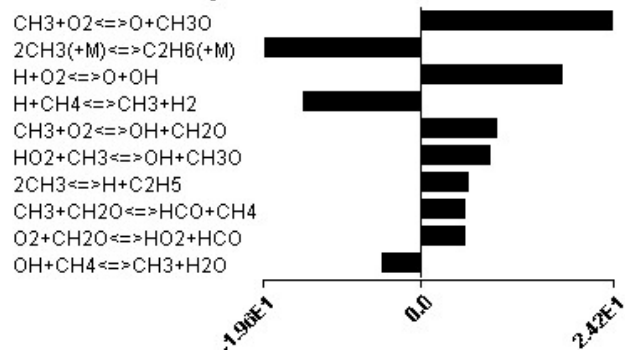


Figure 7: Sensitivity analysis of H.

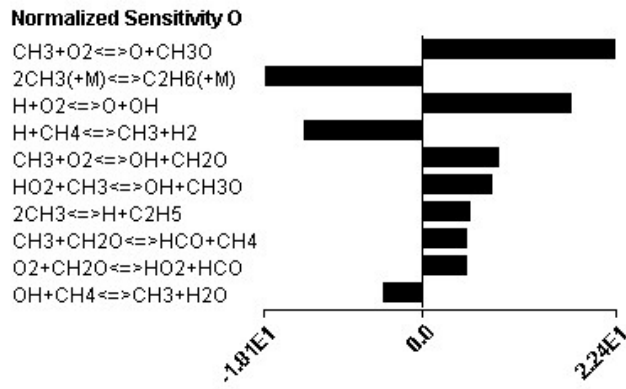


Figure 8: Sensitivity analysis of CH.

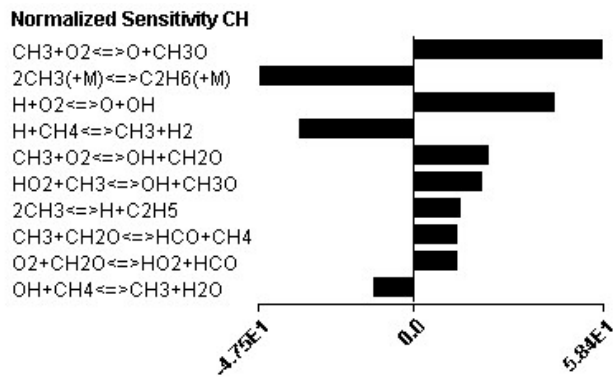


Figure 9: Sensitivity analysis of OH.

At time 0.00116 s corresponding to 1800 K the results of sensitivity analysis for O, H, CH and OH are as follow:

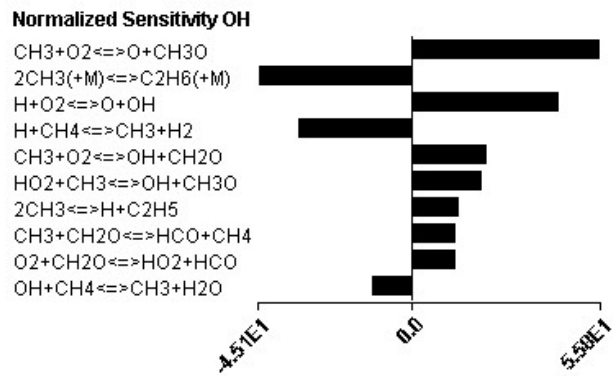


Figure 10: Sensitivity analysis of O.

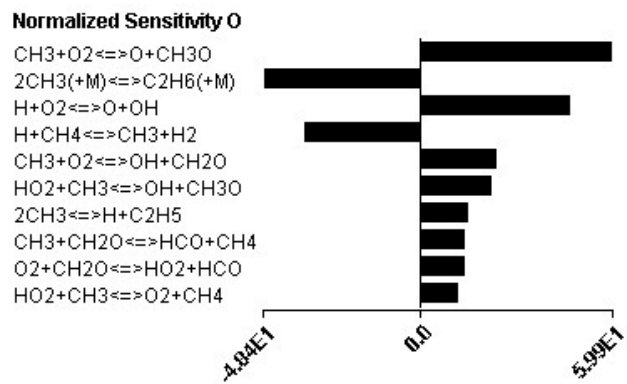


Figure 11: Sensitivity analysis of H.

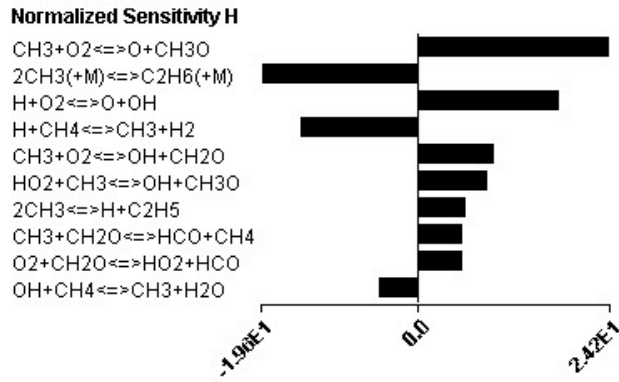


Figure 12: Sensitivity analysis of CH.

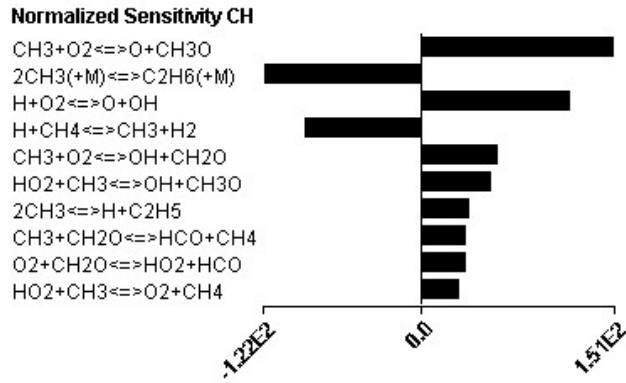


Figure 13: Sensitivity analysis of OH.

75 Fig 14 shows that considering heat transfer will retire the SOC and also will reduce the max cylinder temperature and average temperature in the expansion stage because of energy loss to the cylinder walls.

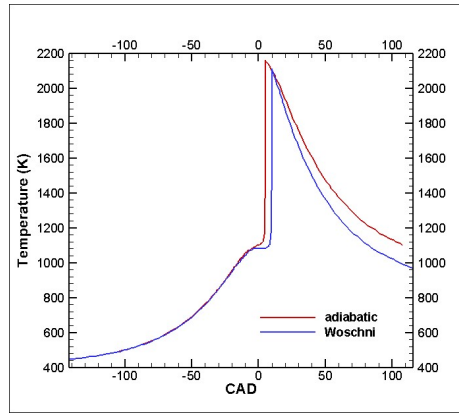


Figure 14: Temperature profile with respect to crank angle degree (CAD).

Based on our simulation results (Fig. 15), considering heat transfer have the same effect on the in-cylinder pressure history.

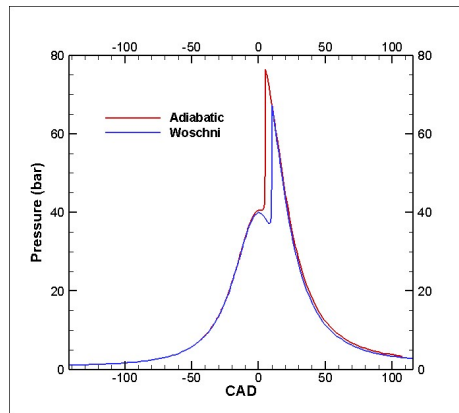


Figure 15: Pressure profile with respect to crank angle degree (CAD).

80 Figs. ?? demonstrate in-cylinder temperature and pressure histories for the n-heptane fueled HCCI engine.

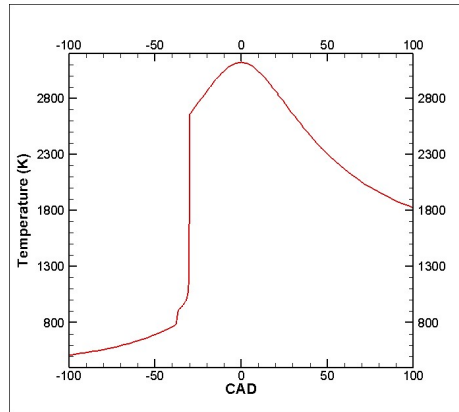


Figure 16: Temperature profile with respect to crank angle degree (CAD).

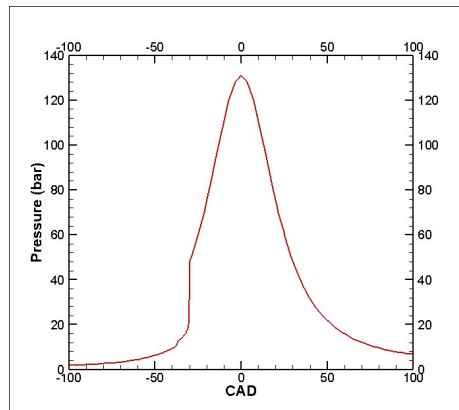


Figure 17: Pressure profile with respect to crank angle degree (CAD).

The effect of engine speed on auto ignition, are demonstrated in Figs. ?? it is found that with increasing the engine speed start of combustion postpones which means there is a longer ignition delay.

85 Figs. ?? demonstrate in-cylinder temperature and pressure histories for the n-heptane fueled HCCI engine.

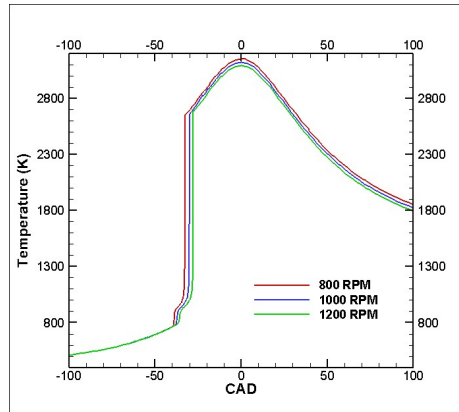


Figure 18: Temperature profile with respect to crank angle degree (CAD).

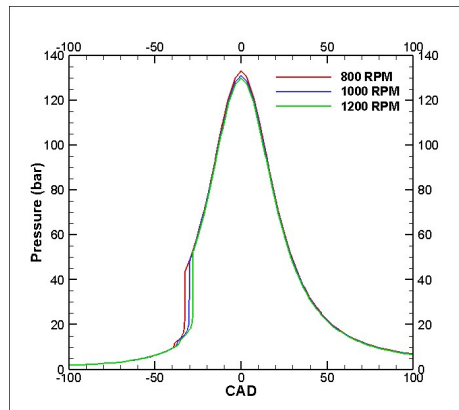


Figure 19: Pressure profile with respect to crank angle degree (CAD).

5. Conclusions

The effects of heat transfer and engine speed on combustion behavior of HCCI combustion engine is investigated and the following conclusions can be derived from this research:

- Considering heat transfer in HCCI simulation causes delay in SOC because of energy loss to the cylinder wall.

- The peak temperature, pressure and also the average temperature and pressure for the expansion stage is reduce. There for we will have smaller engine
95 performance.

- Increasing engine speed (rpm) will cause delay in SOC because of giving less time to the H radicals to react with other species and start the combustion inside the cylinder.

- [1] A. Y. Nobakht, R. K. Saray, A. Rahimi, A parametric study on natural gas
100 fueled hcci combustion engine using a multi-zone combustion model, *Fuel*
90 (4) (2011) 1508–1514.
- [2] S. Onishi, S. H. Jo, K. Shoda, P. Do Jo, S. Kato, Active thermo-atmosphere
combustion (atac)-a new combustion process for internal combustion en-
gines, Tech. rep., SAE Technical Paper (1979).
- [3] P. M. Najt, D. E. Foster, Compression-ignited homogeneous charge com-
105 bustion, Tech. rep., SAE Technical Paper (1983).
- [4] R. K. Maurya, N. Akhil, Numerical investigation of ethanol fuelled hcci
engine using stochastic reactor model. part 2: Parametric study of perfor-
mance and emissions characteristics using new reduced ethanol oxidation
110 mechanism, *Energy Conversion and Management* 121 (2016) 55–70.
- [5] A. Y. Nobakht, R. K. Saray, G. S. Astiar, Optimization of gri-mech 3.0
mechanism using hcci combustion models and genetic algorithm, *Internation-
al Journal of Engineering, Transactions A: Basics* 24 (2) (2011) 155–168.
- [6] H. Mahabadipour, K. K. Srinivasan, S. R. Krishnan, A second law-based
115 framework to identify high efficiency pathways in dual fuel low temperature
combustion, *Applied Energy* 202 (2017) 199–212.
- [7] H. Mahabadipour, K. Srinivasan, S. Krishnan, lost available imep: A
second-law-based performance parameter for ic engines, in: *ASME 2016
Internal Combustion Engine Division Fall Technical Conference*, American
120 Society of Mechanical Engineers, 2016, pp. V001T03A021–V001T03A021.
- [8] J. Eng, W. Leppard, T. Sloane, The effect of pox on the autoignition chem-
istry of n-heptane and isoctane in an hcci engine, Tech. rep., SAE Tech-
nical Paper (2002).
- [9] J. Yang, T. Culp, T. Kenney, Development of a gasoline engine system
125 using hcci technology-the concept and the test results, Tech. rep., SAE
Technical Paper (2002).

- [10] H. Mahabadipour, K. K. Srinivasan, S. R. Krishnan, Characterization of exhaust exergy flows in a diesel engine from the perspective of exhaust waste energy recovery, *Applied Energy*.
- 130 [11] J. Eng, Characterization of pressure waves in hcci combustion, Tech. rep., SAE Technical Paper (2002).
- [12] A. Y. Nobakht, H. Mahabadipour, Cfd simulation of tesla-type microvalves.
- [13] Z. Zheng, M. Yao, Charge stratification to control hcci: Experiments and cfd modeling with n-heptane as fuel, *Fuel* 88 (2) (2009) 354–365.
- 135 [14] X.-C. Lu, W. Chen, Z. Huang, et al., A fundamental study on the control of the hcci combustion and emissions by fuel design concept combined with controllable egr. part 2. effect of operating conditions and egr on hcci combustion, *Fuel* 84 (9) (2005) 1084–1092.
- [15] N. Komminos, D. Hountalas, C. Rakopoulos, A parametric investigation of hydrogen hcci combustion using a multi-zone model approach, *Energy conversion and management* 48 (11) (2007) 2934–2941.
- 140 [16] J. Zheng, J. A. Caton, Use of a single-zone thermodynamic model with detailed chemistry to study a natural gas fueled homogeneous charge compression ignition engine, *Energy conversion and management* 53 (1) (2012) 298–304.
- 145 [17] G. Haraldsson, P. Tunestål, B. Johansson, J. Hyvönen, Hcci combustion phasing in a multi cylinder engine using variable compression ratio, Tech. rep., SAE Technical Paper (2002).
- [18] W. Gardiner, V. Lissianski, Z. Qin, G. Smith, D. Golden, M. FRENKLACH, B. Eiteneer, M. Goldenberg, N. Moriarty, C. Bowman, et al., The gri-mechtm model for natural gas combustion and no formation and removal chemistry, in: 5th Int. Conference on Combustion Technologies for a Clean Environment, 1999.
- 150

- [19] J. Chang, O. Güralp, Z. Filipi, D. N. Assanis, T.-W. Kuo, P. Najt, R. Rask,
155 New heat transfer correlation for an hcci engine derived from measurements
of instantaneous surface heat flux, Tech. rep., SAE Technical Paper (2004).
- [20] J. Yang, J. Martin, Approximate solution one-dimensional energy equation
for transient, compressible, low mach number turbulent boundary layer
flows, *Journal of Heat Transfer* 111 (3) (1989) 619–624.