Effect of Cyclo-Pentane Impurities on the Autoignition Reactivity and Properties of a Gasoline Surrogate Fuel

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Abstract

Surrogate fuels that reproduce the characteristics of full-boiling range fuels are key tools to enable numerical simulations of fuel-related processes and ensure reproducibility of experiments by eliminating batch-to-batch variability. Within the PACE initiative, a surrogate fuel for regular-grade E10 (10%vol ethanol) gasoline representative of a U.S. market gasoline, termed PACE-20, was developed and adopted as baseline fuel for the consortium. Although extensive testing demonstrated that PACE-20 replicates the properties and combustion behavior of the full-boiling range gasoline, several concerns arose regarding the purity level required for the species that compose PACE-20. This is particularly important for cyclo-pentane, since commercial-grade cyclo-pentane typically shows 60% - 85% purity. In the present work, the effects of the purity level of cyclo-pentane on the properties and combustion characteristics of PACE-20 were studied. Chemical kinetic simulations were performed to predict the effects of cyclo-pentane impurities on the properties, octane rating and autoignition reactivity under homogeneous charge compression-ignition conditions of PACE-20. From the numerical results, cyclo-pentane with 85% purity or higher is required to reasonably match both the research octane number and motor octane number of the target gasoline. Finally, homogeneous charge compression ignition engine simulations show that impurities have only a modest effect on reactivity at naturally aspirated conditions, but cyclo-pentane purity is critical to properly replicate the pressure dependency of the reactivity.

Introduction

Various independent agencies predict that, by 2050, the share of fleet with an internal combustion engine onboard (including plugin hybrid vehicles) will continue to be substantial. According to the International energy Agency [1], approximately 400 million light-duty vehicles with internal combustion engines will be sold in the U.S. between 2023 and 2050. Therefore, improving engine efficiency while reducing tailpipe pollutant emissions is critical to achieve rapid greenhouse gas (GHG) reduction of the transportation sector. The U.S. Department of Energy Partnership for Advanced Combustion Engines (PACE) initiative was a national laboratory combustion consortium that included Argonne National Laboratory, Lawrence Livermore National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory and Sandia National Laboratories [2] focused on improving the performance and emissions of internal combustion engines for light-duty applications. Knock mitigation, dilution combustion, and emissions reduction have been identified by the PACE research group as the three main focus areas for light-duty engine research and development.

Within PACE, Cheng et al. [3] developed a surrogate fuel for commercial regular E10 (10%vol ethanol content) gasoline to be used for all the members of the consortium, enabling fuel-related numerical simulations that would not be possible with a full-boiling range fuel and ensuring reproducibility and consistency between results obtained by the different consortium members. This surrogate fuel was termed PACE-20 and is composed by 9 hydrocarbon species representative of the different hydrocarbon classes found in commercial gasoline. The surrogate targeted a research-grade gasoline, termed RD5-87, representative of market regular gasoline in the U.S. [4, 5], and the composition of RD5-87 is compared against that of PACE-20 in Figure 1. Common single component species that are readily obtainable, easy to blend in a lab environment (e.g., that are not a gas at ambient conditions) and have an established chemical kinetic mechanism were used in the surrogate formulation process. An initial surrogate candidate was defined by matching the relative amounts of the different hydrocarbon classes and the carbon number distribution for each hydrocarbon class of RD5-87. Then, the formulation was adjusted in an iterative process until the surrogate satisfied match criteria. Targets used in the formulation of PACE-20 included carbon, hydrogen and oxygen content, distillation characteristics, density, research octane number (RON) and motor octane number (MON), autoignition reactivity at homogeneous charge compression-ignition (HCCI) conditions, and particulate matter index (PMI). This surrogate formulation process is consistent with other methods found in the literature [6, 7], which pointed out the limitations of traditional primary reference fuels (PRF) and toluene primary reference fuels (TPRF) to reproduce the combustion behavior of full-boiling range gasoline fuels [8]. The main properties of both RD5-87 and PACE-20 are shown in Table 1.

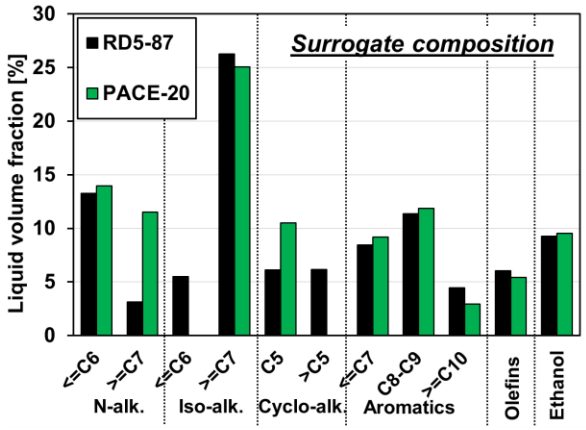

Figure 1. Composition of RD5-87 (from a detailed hydrocarbon analysis) and PACE-20.

PACE-20 has been extensively validated within PACE. The laminar flame speed of PACE-20 [9] and its autoignition reactivity and heat release rate in a rapid compression machine [3] match those of RD5-87. Fuel vaporization and spray development of PACE-20 has been also validated against RD5-87 at canonical spray experiments, including free spray development and morphology [10] and wall impingement and fuel film formation [11]. Engine experiments and simulations have been performed to validate PACE-20 for spray behavior, spray collapse, flash boiling and mixture formation [12–

14]. Combustion behavior of PACE-20 has been also validated against RD5-87 in HCCI engine [3] and spark-ignition (SI) engine experiments [15]. Finally, PACE-20 has been also validated for soot formation under pyrolysis and oxidative conditions [16]. When blending a batch of PACE-20 for laboratory testing, concerns arose regarding how the purity level of the species that compose PACE-20 may affect the accuracy of the surrogate fuel. This is particularly important for cyclo-pentane, since commercial-grade cyclo-pentane typically shows 60% - 85% purity with the two most common impurities in cyclo-pentane being 2,2 dimethyl-butane [17] and iso-pentane [18]. Fuel blending effects on RON and MON have been widely investigated for gasoline [19, 20] and gasoline surrogates [21, 22]. However, to the authors' knowledge, the effect of fuel purity on the performance of a surrogate fuel has not been investigated before, which is particularly important for reducing uncertainties in the experimental evaluation of a surrogate and for performing an adequate comparison between different experimental results. In this short communication, the effects of the purity level of cyclo-pentane on the properties and combustion characteristics of PACE-20 are investigated.

Table 1. Main properties of RD5-87 and PACE-20.

	RD5-87	**PACE-20**
Molecular formula	$C_{6.13}H_{12.07}O_{0.20}$	$C_{5.92}H_{11.62}O_{0.19}$
H/C ratio	1.969	1.964
O/C ratio	0.032	0.032
A/F_{stoich} ratio	14.070	14.086
MW [g/mol]	88.95	85.41
LHV [MJ/kg]	41.770	41.705
Density at 15°C [kg/L]	0.750	0.742
RON	92.3	92.1
MON	84.6	84.5
Antiknock Index (AKI)	88.4	88.3
Sensitivity	7.7	7.6
Carbon [wt %]	82.67	82.90
Hydrogen [wt %]	13.66	13.57
Oxygen [wt %]	3.67	3.53
PMI [-]	1.68	1.51

Methodology

Chemical kinetic simulations were performed to predict the effects of cyclo-pentane impurities on the octane rating and autoignition reactivity under HCCI conditions of PACE-20. Simulations were performed using ANSYS CHEMKIM-PRO software. Two different reactors are used in this work. First a 0-dimensional, closed, homogeneous reactor is used to simulate autoignition of the end-gas and predict the octane rating of the fuel. Second, a 0-dimensional internal combustion engine reactor was used to study the reactivity under HCCI conditions.

A detailed chemical kinetic mechanism for gasoline surrogates from Lawrence Livermore National Lab (LLNL) is used in the simulations [23]. This mechanism includes the chemistry of multiple normal-, iso- and cyclo-alkanes, olefins, aromatics and oxygenated species typically found in gasoline-like fuels, as well as a detailed description of NOx chemistry. The mechanism is composed by 4212 species and 19134 reactions and is an updated version of the free-access chemical kinetic mechanism available on the LLNL website [24], which has been widely validated against experimental data [25].

The RON and MON of the fuel are estimated with a correlation based on the ignition delay under RON-like and MON-like conditions [26]. The experimental pressure and temperature trajectory of the RON (or MON) test is imposed in a closed, homogeneous reactor. This way, the compression effects of both the piston and the flame on the autoignition of the end gas are included in the simulation. The temperature evolution is calculated in the model by solving the energy equation (included source/sink terms from chemical activity) and the volume evolution is obtained to satisfy the equation of state (so the volume of the reactor is constrained, but not constant). The ignition delay obtained in the simulation is correlated with the RON (or MON) numbers, with the correlation determined based on similar computations for fuels with known composition, RON and MON. A total of 56 single-component fuels and primary reference fuel blends were used in the correlation, including n-alkanes, iso-alkanes, cyclo-alkanes, olefins, aromatics, alcohols and other oxygenates, and leading to a coefficient of determination (R^2) of 0.9914. Validations of this method and its application to formulate surrogate fuels can be found in [3, 26, 27].

The Sandia Low-Temperature Gasoline Combustion (LTGC) research engine facility is simulated by a 0-dimensional internal combustion engine reactor. The facility consists of a 0.98L single-cylinder engine (102 mm bore x 120 mm stroke) equipped with a custom piston that provides an open combustion chamber. Fully-premixed HCCI operation was simulated at compression ratio (CR) = 16:1 and 1200 rpm. This facility has been simulated in multiple previous investigations [3, 28, 29], so a detailed description is avoided for brevity's sake. The initial crank angle for the simulations was set at 180 CAD (bottom dead center, BDC), and computations were performed until 420 CAD (exhaust valve opening). The BDC pressure in the simulations was specified to match the experimental data. Heat transfer losses were simulated using Woschni correlation with a wall temperature equal to the experimentally measured fire-deck temperature and with the correlation coefficients adjusted so the simulation reproduced the pressure-temperature trajectory of the experiments before the start of combustion. A validation of the model can be seen in references [29–33].

PACE-20, with a composition derived from ideally pure elements as detailed in Table 2, is artificially contaminated with 2,2 dimethyl-butane and iso-pentane to simulate the effect of cyclo-pentane impurities on the fuel. More specifically, the cyclo-pentane content of PACE-20 is replaced by blends of 70% cyclo-pentane (CPT) + 30% 2,2 dimethyl-butane (NEC6), 70% CPT + 30% iso-pentane (IC5), and 85% CPT + 15% NEC6, which represent the composition of commercial-grade cyclo-pentane with 70% purity and 85% purity, respectively [17, 18].

Table 2. Composition of PACE-20 in liquid volume fractions.

N-pentane	13.95%
N-heptane	11.53%
Iso-octane	25.05%
Cyclo-pentane	10.50%
1-Hexene	5.41%
Toluene	9.19%
1,2,4 Trimethylbenzene	11.87%
Tetralin	2.95%

Ethanol	9.55%

Mixing blending rules were used to estimate the carbon and hydrogen content, density, lower heating value and heat of vaporization of PACE-20 with and without impurities. The Lee-Keser equation [34] is used to estimate the vapor pressure of the individual species that compose the surrogate, whereas Raoult's law is used to calculate the vapor pressure of the fuel blends. The particulate matter index is predicted based on the vapor pressure and double bond equivalent of the fuel as in [35]. Finally, RON and MON are obtained via CHEMKIN-PRO simulations as explained above.

Table 3. Properties of straight PACE-20 and PACE-20 with 85% pure and 70% pure cyclo-pentane.

	100% CPT	**85% CPT 15% NEC6**	**70% CPT 30% NEC6**	**70% CPT 30% IC5**
H/C ratio	1.964	1.971	1.978	1.978
O/C ratio	0.0320	0.0318	0.0317	0.0319
A/F_{stoich} *ratio*	14.086	14.065	14.076	14.072
MW [g/mol]	85.41	85.94	86.25	85.70
LHV [MJ/kg]	41.705	41.932	42.095	41.940
Density at 15°C [kg/L]	0.742	0.743	0.743	0.737
P_{vapor} *at 38°C [kPa]*	32.9	32.7	32.6	35.6
HOV [kJ/kg]	419.9	419.5	419.0	418.0
PMI [-]	1.51	1.507	1.504	1.506

Results and discussion

Fuel properties and octane rating

Table 3 shows the main fuel properties of straight PACE-20 and PACE-20 with 85% pure and 70% pure cyclo-pentane. Cyclo-pentane impurities barely affect the physical properties of the fuel, and the deviation between PACE-20 and the blends with cyclo-pentane impurities is lower than ±1% for all cases except for the vapor pressure of 70% CPT + 30% IC5. The volatility of iso-pentane is much higher than that of cyclo-pentane and, as a result, the vapor pressure of PACE-20 with 70% CPT + 30% IC5 is 8% higher than that of straight PACE-20. This deviation may have some impacts on fuel vaporization and spray collapse propensity so using cyclo-pentane with iso-pentane impurities is not recommended.

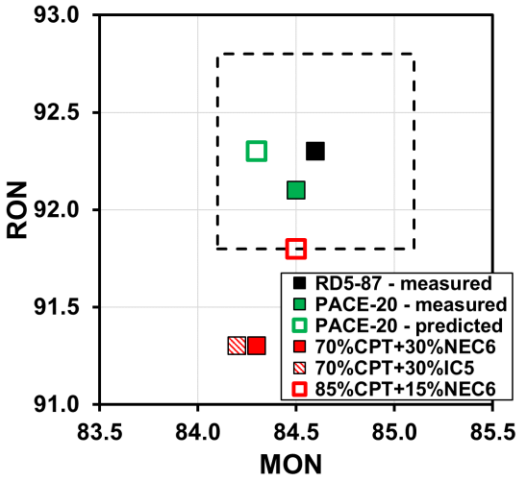

Figure 2. Measured RON and MON of RD5-87 and PACE-20, and predicted RON and MON of straight PACE-20 and PACE-20 with 85% and 70% pure cyclo-pentane.

Figure 2 shows the measured RON and MON of RD5-87 and PACE-20 and the predicted RON and MON for straight PACE-20 and PACE-20 with 85% pure and 70% pure cyclo-pentane. The predicted octane rating of PACE-20 is in good agreement with the measured value (within ± 0.2 units), giving confidence on the RON and MON simulations. Cyclo-pentane impurities tend to decrease the RON of the surrogate, and both PACE-20 blends with 70% pure cyclo-pentane (70% CPT + 30% NEC6 and 70% CPT + 30% IC5) show relatively large deviations in RON compared to the target fuel (approx. 1.0 units in both cases). Interestingly, cyclo-pentane impurities only show a mild effect on the MON of the surrogate. As a result, the octane sensitivity (defined as S = RON – MON) decreases due to impurities. This may be explained by the blending octane rating of cyclo-pentane compared to that of the impurities [36]. The blending RON of cyclo-pentane (BRON = 141) is approx. 40 units higher than that of 2,2 dimethyl-butane (BRON = 99) and iso-pentane (BRON = 100). However, the blending MON of cylo-pentane (BMON = 123) is approx. 20 units higher than that of 2,2 dimethyl-butane (BMON = 99) and iso-pentane (BMON = 104). This is because cyclo-pentane is a very effective suppressor of the low-temperature chemistry of fuel blends, and low-temperature chemistry is more important at RON-like conditions than at MON-like conditions. Thus, cyclo-pentane impurities tend to decrease both the RON and the MON of the blend, but RON will be more affected than MON. Assuming an acceptable deviation for RON and MON of 0.5 units (represented by the dashed square in the figure), all PACE-20 blends show acceptable MON values but only PACE-20 with 85% pure cyclo-pentane has both RON and MON within the acceptable range.

Autoignition reactivity under engine conditions

Two HCCI engine simulation campaigns were performed with straight PACE-20 and PACE-20 with 85% and 70% pure cyclo-pentane. The first campaign consisted of a combustion timing sweep (represented by the 50% burn point, CA50) by varying the temperature at intake valve closing (IVC) at intake pressure of 1.0 bar and equivalence ratio of 0.40 with no EGR. The second campaign consisted of an intake pressure sweep at IVC temperature of 60°C and equivalence ratio of 0.38 in which the EGR rate was adjusted to keep the CA50 constant and equal to 373 CAD.

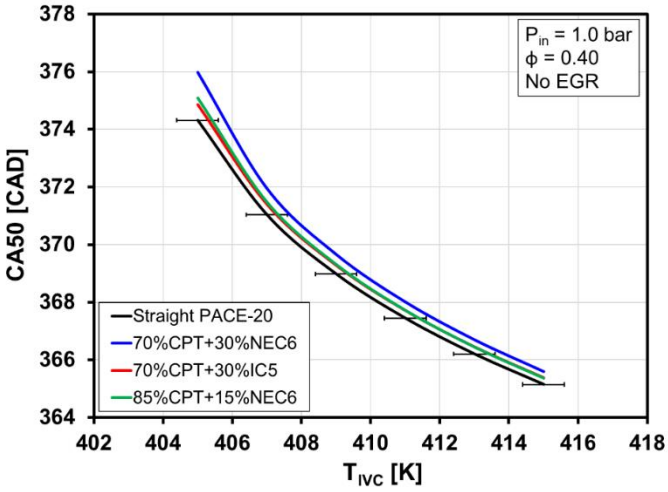

Figure 3. CA50 sweep vs. TIVC for straight PACE-20 and PACE-20 with 85% and 70% pure cyclo-pentane.

Figure 3 shows the results for the CA50 sweep at naturally aspirated conditions. Error bars represent the typical repeatability achievable in the engine facility [3]. As expected, the CA50 advances as the intake temperature increases because the ignition delay of the fuel decreases, advancing the ignition. Similar trends are seen for all fuels. PACE-20 with 85% CPT + 15% NC6 and PACE-20 with 70% CPT + 30% IC5 give nearly identical results, and their performance is similar to that of straight PACE-20 (within expected experimental repeatability). PACE-20 with 70% CPT + 30% NEC6 is slightly less reactive than straight PACE-20 (at a given IVC temperature, it shows a more retarded CA50 than straight PACE-20), but the agreement is still very good. Results suggest that impurities have only a modest effect on the autoignition reactivity at naturally aspirated conditions.

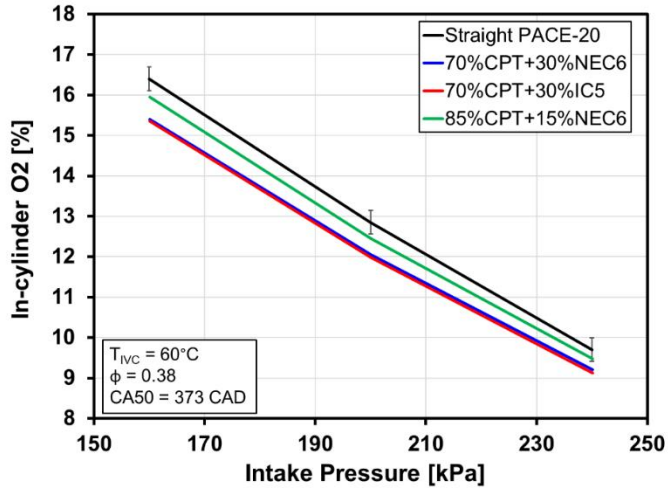

Figure 4. CA50 sweep vs. TIVC for straight PACE-20 and PACE-20 with 85% and 70% pure cyclo-pentane.

Figure 4 shows the in-cylinder oxygen level required to keep the CA50 equal to 373 CAD during the intake pressure sweep described before. The error bars for the straight PACE-20 series represent the typical repeatability achievable in the engine facility [3]. The ignition delay of the fuel decreases as the intake pressure increases, which tends to advance the CA50. On the other hand, the ignition delay of the fuel increases as the in-cylinder oxygen content decreases, which tends to retard the CA50. Thus, as the intake pressure increases, less in-cylinder oxygen (more EGR) is required to keep the CA50 constant [37]. Cyclo-pentane impurities tend to make the fuel more reactive (at a given intake pressure, PACE-20 blends with impurities require less oxygen than straight PACE-20). The deviation between straight PACE-20 and PACE-20 with 85% CPT + 15% NC6 is not large and almost within the expected experimental repeatability. However, both PACE-20 with 70% CPT + 30% NEC6 and PACE-20 with 70% CPT + 30% IC5, which give nearly identical results, show significantly higher reactivity than straight PACE-20. Results suggest that cyclo-pentane is a key species to properly reproduce the pressure-dependency of PACE-20 autoignition reactivity, and cyclo-pentane with ≥ 85% purity is recommended for experiments at high pressure conditions.

Summary and conclusions

In this short communication, the effects of cyclo-pentane impurities on the physical properties, octane rating and HCCI autoignition reactivity of a gasoline surrogate fuel, PACE-20, were analyzed. Impurities barely affect the physical properties of the fuel except for cyclo-pentane with iso-pentane impurities, which tends to increase the vapor pressure of the surrogate fuel up to 8% for 70% pure cyclo-pentane. Thus, using cyclo-pentane with iso-pentane impurities is not recommended. Impurities only affect the MON of the fuel mildly. However, cyclo-pentane with 85% purity or higher is required to reasonably match the RON of the fuel. Impurities only have a modest effect on fuel's reactivity at naturally aspirated HCCI engine conditions. For boosted operation, cyclo-pentane with 85% purity matches the changes in reactivity with increased boost with reasonable accuracy, whereas cyclo-pentane with 70% purity is significantly more reactive than the straight fuel. In conclusion, using cyclo-pentane with at least 85% purity for surrogate fuel blending is recommended, with impurities composed by 2,2 dimethyl-butane preferred over iso-pentane.

References

[1] "Annual Energy Outlook 2023 - U.S. Energy Information Administration (EIA)." [Online]. Available: https://www.eia.gov/outlooks/aeo/index.php. [Accessed: 25-Sep-2023].

[2] I. Ekoto, M. J. McNenly, P. Miles, S. Sibendu, and J. P. Szybist, "Partnership for Advanced Combustion Engines (PACE) – A Light-Duty National Laboratory Combustion Consortium," presented at the U.S. Department of Energy Vehicle Technologies Office 2021 Annual Merit Review and Peer Evaluation Meeting, Washington, D.C., 2021.

[3] S. Cheng *et al.*, "Replicating HCCI-like autoignition behavior: What gasoline surrogate fidelity is needed?," *Applications in Energy and Combustion Science*, vol. 12, p. 100091, Dec. 2022.

[4] D. Lopez Pintor, G. Gentz, and J. Dec, "Mixture Stratification for CA50 Control of LTGC Engines with Reactivity-Enhanced and Non-Additized Gasoline," *SAE Technical Paper 2021-01-0513*, Apr. 2021.

[5] D. Lopez Pintor and J. E. Dec, "Development and Evaluation of Surrogates for Distillate Gasolines as Applied to RD5-87," *US DOE Advanced Engine Combustion Working Group Meeting*, Aug. 2020.

[6] A. Bhattacharya, O. Kaario, V. Vuorinen, R. Tripathi, and T. Sarjovaara, "Analysis of Gasoline Surrogate Combustion Chemistry with a Skeletal Mechanism," presented at the SAE Powertrains, Fuels & Lubricants Meeting, 2020.

[7] F. Kaliafetis and D. R. F. Cracknell, "Explicit equations for designing surrogate gasoline formulations containing ethanol, isopentane, n-heptane, isooctane and toluene," presented at the 2023 JSAE/SAE Powertrains, Energy and Lubricants International Meeting, Kyoto, Japan, 2023.

[8] A. Ahmed, G. Goteng, V. S. B. Shankar, K. Al-Qurashi, W. L. Roberts, and S. M. Sarathy, "A computational methodology for

formulating gasoline surrogate fuels with accurate physical and chemical kinetic properties," *Fuel*, vol. 143, pp. 290–300, Mar. 2015.
[9] S. W. Wagnon *et al.*, "Chemical Kinetic Models for Surrogate Fuels," *2021 DOE Vehicle Technologies Office Annual Merit Review Presentation - Project ID# ace139*, Jun. 2021.
[10] C. Powell *et al.*, "Fuel Injection and Spray Research," presented at the U.S. Department of Energy Vehicle Technologies Office 2021 Annual Merit Review and Peer Evaluation Meeting, Washington, D.C., 2021.
[11] L. M. Pickett *et al.*, "Spray Wall Interactions," presented at the U.S. Department of Energy Vehicle Technologies Office 2021 Annual Merit Review and Peer Evaluation Meeting, Washington, D.C., 2021.
[12] K. D. Edwards, M. Wissink, G. Jatana, F. Chuahy, and S. Curran, "Cold-start Modeling and Experiments for Emissions Reduction," presented at the U.S. Department of Energy Vehicle Technologies Office 2021 Annual Merit Review and Peer Evaluation Meeting, Washington, D.C., 2021.
[13] R. Torelli, H. Guo, S. Som, M. Sjöberg, N. Kim, and D. Reuss, "Spray/Flow Interaction in Engines," presented at the U.S. Department of Energy Vehicle Technologies Office 2021 Annual Merit Review and Peer Evaluation Meeting, Washington, D.C., 2021.
[14] N. Kim, D. L. Reuss, and M. Sjöberg, "Assessment of an E10 gasoline surrogate: Qualitative and quantitative comparisons of in-cylinder spray morphology," *International Journal of Engine Research*, Feb. 2023.
[15] J. Kim, M. Ameen, R. Scarcelli, N. Kim, E. Singh, and M. Sjöberg, "Evaluation of Spray and Combustion Models for Simulating Dilute Combustion in a Direct-Injection Spark-Ignition Engine," *J. Eng. Gas Turbines Power*, vol. 145, no. 8, Aug. 2023.
[16] J. Manin *et al.*, "Soot Modeling and Experiments," presented at the U.S. Department of Energy Vehicle Technologies Office 2021 Annual Merit Review and Peer Evaluation Meeting, Washington, D.C., 2021.
[17] "Cyclopentane OmniSolv® - EMD Millipore Trademark Products - Chemicals." [Online]. Available: https://www.taylorscientific.com/cyclopentane-omnisolvr. [Accessed: 09-Oct-2023].
[18] INEOS Oligomers, "Cyclopentane 70 - Sales Specification." 2016.
[19] G. Bourhis, J.-P. Solari, V. Morel, and R. Dauphin, "Using Ethanol's Double Octane Boosting Effect with Low RON Naphtha-Based Fuel for an Octane on Demand SI Engine," *SAE International Journal of Engines*, vol. 9, no. 3, pp. 1460–1474, Apr. 2016.
[20] D. Vuilleumier and M. Sjöberg, "Significance of RON, MON, and LTHR for Knock Limits of Compositionally Dissimilar Gasoline Fuels in a DISI Engine," *SAE International Journal of Engines*, vol. 10, no. 3, pp. 938–950, Mar. 2017.
[21] A. Reddy Vallapureddy, H. Zhuang, J. Li, D. DelVescovo, C. P. Kolodziej, and A. Hoth, "Defining the Boundary Conditions of the CFR Engine under MON Conditions, and Evaluating Chemical Kinetic Predictions at RON and MON for PRFs," presented at the SAE WCX Digital Summit, 2021.
[22] L. Knuutila, O. Kaario, M. Larmi, A. Santasalo-Aarnio, A. Karvo, and U. Kiiski, "Blending Behavior of Hydrocarbon and Oxygenate Molecules to Optimize RON and MON for Modern Spark-Ignition Engines (SI)," presented at the SAE Powertrains, Fuels & Lubricants Meeting, 2020.
[23] M. Mehl *et al.*, "A Comprehensive Detailed Kinetic Mechanism for the Simulation of Transportation Fuels," *US Sections of the Combustion Institute*, 2017.
[24] M. Mehl, W. J. Pitz, C. K. Westbrook, and H. J. Curran, "Kinetic modeling of gasoline surrogate components and mixtures under engine conditions," *Proceedings of the Combustion Institute*, vol. 33, pp. 193–200, 2011.
[25] M. Mehl, W. J. Pitz, C. K. Westbrook, K. Yasunaga, C. Conroy, and H. J. Curran, "Autoignition behavior of unsaturated hydrocarbons in the low and high temperature regions," *Proceedings of the Combustion Institute*, vol. 33, pp. 201–208, 2011.
[26] C. K. Westbrook, M. Sjöberg, and N. P. Cernansky, "A new chemical kinetic method of determining RON and MON values for single component and multicomponent mixtures of engine fuels," *Combustion and Flame*, vol. 195, pp. 50–62, Sep. 2018.
[27] A. Cuoci *et al.*, "Simulating combustion of a seven-component surrogate for a gasoline/ethanol blend including soot formation and comparison with experiments," *Fuel*, vol. 288, p. 119451, Mar. 2021.
[28] G. Guleria, D. Lopez Pintor, J. E. Dec, and D. Assanis, "A comparative study of gasoline skeletal mechanisms under partial fuel stratification conditions using large eddy simulations," *International Journal of Engine Research, paper no. 14680874*, 2021.
[29] S. Cho and D. Lopez Pintor, "Understanding the effects of doping a regular E10 gasoline with EHN in an HCCI engine: Experimental and numerical study," *Fuel*, vol. 329, p. 125456, Dec. 2022.
[30] M. Sjöberg and J. E. Dec, "An Investigation of the Relationship Between Measured Intake Temperature, BDC Temperature, and Combustion Phasing for Premixed and DI HCCI Engines," presented at the 2004 SAE Fuels & Lubricants Meeting & Exhibition, 2004, pp. 2004-01–1900.
[31] J. E. Dec, W. Hwang, and M. Sjöberg, "An Investigation of Thermal Stratification in HCCI Engines Using Chemiluminescence Imaging," *SAE Technical Paper 2006-01-1518*, 2006.
[32] D. Lopez-Pintor, J. Dec, and S. Cho, "Performance of octane index in LTGC engines from beyond MON to beyond RON," *Fuel*, vol. 341, p. 127625, Jun. 2023.
[33] D. Lopez Pintor and J. E. Dec, "Development and validation of an EHN mechanism for fundamental and applied chemistry studies," *SAE Int. J. Adv. & Curr. Prac. in Mobility*, vol. 4, no. 4, pp. 1198–1216, 2022.
[34] B. I. Lee and M. G. Kesler, "A generalized thermodynamic correlation based on three-parameter corresponding states," *AIChE Journal*, vol. 21, no. 3, pp. 510–527, 1975.
[35] M. Fatouraie *et al.*, "Investigation of the Impact of Fuel Properties on Particulate Number Emission of a Modern Gasoline Direct Injection Engine," presented at the WCX World Congress Experience, 2018, pp. 2018-01–0358.
[36] A. P. I. R. Project 45, "Knocking characteristics of pure hydrocarbons," *ASTM Special Technical Publication No. 225*, 1958.
[37] J. E. Dec, Y. Yang, and N. Dronniou, "Boosted HCCI - Controlling Pressure-Rise Rates for Performance Improvements using Partial Fuel Stratification with Conventional Gasoline," *SAE Int. J. Engines*, vol. 4, no. 1, pp. 1169–1189, 2011.