Development of a Multi-component Surrogate Model for Diesel Combustion at High Temperatures via Extension of the Naphthene Model

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Abstract

Diesel fuel is widely used in transportation sections worldwide, such as in road- and railway, as well as in aviation. Despite its importance, the number of existing theoretical studies focused on its combustion characterization, particularly on kinetic surrogate modeling, remained limited. This issue became the topic of recent researches of us. The recently published diesel surrogate model by the authors consists of a semi-detailed kinetic model and three surrogate formulas, including four components, namely: n-dodecane, iso-octane, toluene and cyclohexane, with various mole fractions. As found in previous research, the high-temperature reactions of cyclohexane, as the simplest naphthene molecule available, play important roles in determination of the high-temperature combustion behavior of the surrogate blends. Specifically important were the cascading dehydrogenation reactions of cyclohexane in prediction of ignition delay time data, and formation of the poly aromatic hydrocarbons. Due to this fact, in current research the cyclohexane will be replaced by propyl-cyclohexane, which has more complex molecular structure and larger size, and therefore is known as a more realistic substitution for naphthenic compound found in diesel blends. To this aim, the introduced surrogate formulas will be updated for high temperature ranges, and the corresponding kinetic model will be further extended, using the latest published naphthene sub-model. The simulation results will be compared with the experimental data, namely the high temperature ignition delay time and laminar flame speed data, as well as with the results of previous model. Since the performance of basis model was very consistent with ignition delay time data, the initial goal of this research is identified as repeating the same model response after substitution of propyl-cyclohexane. On this basis, a new surrogate formula will be introduced. Moreover, the appeared changes in prediction of laminar flame speed data will be in detailed discussed. At the end, the effective pathway toward formation of poly aromatic species will be investigated at the high temperatures.

Keywords: *Diesel Combustion, Diesel Surrogate Model, Naphthenes*

Nomenclature

CHX – Cyclohexane
PCHX – Propyl-cyclohexane
PAH – Poly-Aromatic Hydrocarbons
BAPYR – Benzo[A]Pyrene
HC – Hydrocarbon Classes
DCN – Derived Cetane Number
F-76 – primary naval fuel
HRD-76 – Algae-based diesel fuel
ULSD#2 – Ultra-low-sulfur diesel

FD9A –FACE Diesel #9
Stage V-VI – European Stage V-Vi Non-Road Emission Standars
SRG – Surrogate Fuel
JFS – Jet Fuel Surrogate
DFS – Diesel Fuel Surrogate
HT- High Temperature
LT – Low Temperature

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1. Introduction

Among the conventional fuels used in transportation, diesel fuel has a particular place, due to its wide range of usage in rail and road transportation, but also in aviation. Particularly the F-76 and the HRD-76 biodiesel blends, which are widely in use in civil, as well as military fighter jets. This is mainly due to the high heating value and the reactive character of the fuels, the procedure of the production, the final market price, and ease of access worldwide compared with other energy carriers, which make diesel an attractive choice. Besides that, diesel is more preferred over the other liquid fuels, due to its lower contamination and corrosion level, and therefore, less maintenance costs [1].

Conventional fuels, such as diesel and jet blends are usually composed of hundreds of different hydrocarbons, each producing different intermediate species during the combustion. A modeling concept, known as the Surrogate Model, are commonly used in the past decade, in order to model different blends. Despite of their conceptual simplicity, the surrogate modeling has many hidden aspects which increases the complexity and therefore the final model uncertainties, which were extensively discussed in our previous research [2].

The first challenge in this way is that the conventional diesel blends have different compositions, and thus, different thermo-chemical properties. Therefore, setting the desired target fuel properties is the first step. There are several worldwide famous diesel blends with fossil basis such as F-76, ULSD No.2, Stage V-VI, with known thermos-chemical properties and hydrocarbon distribution, but also there are some gasoil mixtures, which might still need to go through fuel standardization and experimental characterization procedure, see Table 1. Besides that, there is a matter of discrepancies and uncertainties between the outcomes of the models, as well as the model validation procedures.

The other challenge is the issue of surrogate modelling and adjustment of the proper of hydrocarbon classes together with their corresponding fractions in the surrogate compositions. An accurate surrogate mixture must be adjust in such way that, it can successfully reflect the physical, as well as the chemical properties of the real fuel.

Table 1. Comparison of cetane number and compositions of different diesel blends [3].

Property/Composition	F-76 [4]	HRD-76 [4]	ULSD#2 [5]	FD9A [5]	Stage-V [6]	Stage-VI [6]
DCN	48.8	78.5	43.7	44.2	54.9	52.8
Saturates (weight%)	79	99	69.85	62.6	83.8	84.2
n –Alkanes	54	48	16.38	10.26	49.2	40.4
Iso-Alkanes	19	51	18.44	23.4	-	-
Cycloalkanes	6	~0	35.3	28.94	34.6	43.8
Aromatics (weight%)	16	~0	30.05	36.43	16.2	15.8

DCN: Derived Cetane Number, by ASTM D6890; **F-76:** primary naval fuel, also known as Fuel, Naval Distillate; **HRD-76:** Algae-based diesel fuel; **ULSD#2:** Ultra-low-sulfur diesel; **FD9A:** FACE Diesel #9; **Stage V-VI :** European Stage V-Vi Non-Road Emission Standars

## 2. A Review Over The Well- Stablished Diesel Surrogates Models

In early studies, n-heptane (C_7H_{16}) was often considered as average surrogate composition for diesel [7]. This choice was mainly due to their similar DCN. However, the mechanism of n-heptane does not reflect several important aspects of diesel combustion process and thus, it led to significant model uncertainties, particularly in the case of the amount of heat release [8, 9, 10, 11]. Additionally, the pollutants, resulting by n-heptane combustion procedure is fundamentally different from diesel, particularly in the case of soot formation and its precursors, which is very important in the case of

HiSST-2024-0073
Development of a Multi-component Surrogate Model for Diesel Combustion at High Temperatures via Extension of the Naphthene Model

Page | 2

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studying diesel combustion [12]. Pitz and Mueller [13] argued that a proper surrogate composition should include the necessary hydrocarbon classes namely: n-alkanes, iso-alkanes, cyclo-alkane, and aromatics in order to have the desired uncertainty. There are several conducted studies focused on multi-components (3-5 components) surrogate modeling. Table 2 summarizes these models alongside with the input formula, and general information about their kinetic model and the mean of validation. It is observed that, most of the listed models used reduced kinetic mechanisms. The reduced mechanisms are advantageous since they enable us with higher speed of calculation. On the other side, they are normally accompanied with significant level of uncertainty, since the reduced models are usually only consistent with their target data, and less accurate on the rest of the available datasets. More else, the published models, except the most recent one [2], are not enhanced with the newly published sub-mechanisms, such as naphthenes, C_0-C_3 chemistry, and PAH sub-models, which definitely play important roles in prediction power of overall model, particularly on describing the the ignition behavior, flame specifications, and formation of PAHs as the main precursors for soot. Here it is worth to mention that, although many of mentioned models introduced a surrogate formula with an aromatic component, there no adequate studies available focusing on PAH formation through diesel combustion.

Table 2. A review over the main published surrogate models for diesel blends in literature.

Reference	Surrogate Formula	Kinetic Mechanism	Validation Medium
Naik et al. 2010 [6]	4 components TDCN/ DCAN/ HMN/ AMN	DM: 3800/ 15000 (sp/ react) RM: 436 species	JSR (SpC) [14]
Ra & Reitz 2010 [15]	4 components TDCN/ TLN/ CHX/ HPN	RM: MultiChem	ST (IDT) [16] Engine Exp. [17]
Chang et al. 2015 [18]	4 components DCAN/ IOCT/ MCHX/ TLN	RM: 70/ 220 (sp/ react)	ST (IDT) [19, 20] JSR (SpC) [14, 21] CF (LFS) [22]
Yu et al. 2018 [23]	5 components DDCAN/ HMN/ IOCT/ TLN/ DCL	RM: 74/ 189 (sp/ react)	ST (IDT) [4, 24] JSR (SpC) [14] CF (LFS) [22]
Bai et al. 2020 [25]	3 components HXN/ HMN/ AMN	RM: 74/ 189 (sp/ react)	RCM (IDT) [5, 26, 27] ST (IDT) [4, 28, 29] JSR (SpC) [14, 21] CF (LFS) [22, 30]
Abbasi et al. 2023 [2]	4 components DCAN/ IOCT/ CHX/ TLN	DM: 170/ 1024 (sp/ react)	RCM (IDT) [5, 26, 27] ST (IDT) [4, 28, 29] CF (LFS) [22]

In previous researches of the author [2] a multi-component surrogate formula, including: n-Dodecane, iso- Octane, Cyclohexane, and Toluene, alongside with the corresponding kinetic model was developed. The model development proceeded through modification of the JFS of [43] by adding the recent C_0-C_3 [31], PAH [32, 33] and CHX [34, 35] sub-models. Three surrogate mixtures (SRG1-3) with different hydrocarbon distributions were introduced (Fig 1), which have been used to simulate the selected IDT and LFS data.
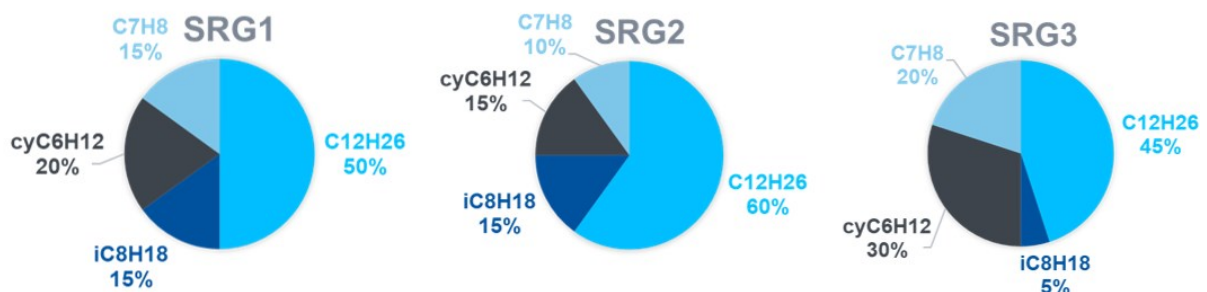
Fig 1. Introduced Diesel Surrogates in [2].

This surrogate model was successfully validated versus the experimental values, particularly in the case of IDT data within HT ranges, where the ultimate results where in perfect accordance with experimental data. The model was very successful in prediction of the LT ignition related phenomena, such cool flame, early ignition, and NTC region over the vast initial temperatures, different mixture fractions and

pressure ranges. The simulation results of LFS data by all SRGs reveals an underestimation, where the position of the maximum flame speed was foreseen at φ=1.2, which is shifted towards the fuel-rich zone compared with experimental data. Finally, the results of ROPAD analysis revealed the important role of the CHX sub-mechanism in controlling the PAH formation, particularly in lower temperature ranges, which emphasizes on importance of naphtanes sub-mechanism.

Cyclohexane is known as basic naphthenic compound, which is normally used in many surrogate models. This widely use of CHX is due to its simple structure, but also due this fact that it is the mostly studied naphthene. However, in reality the naphthenic compounds found in convenient fuel blends, such as diesel and jet fuels are more complex.

Therefore, in order to increase the model capability on naphthene's sub-model, it is tried to replace the CHX contribution in the surrogate formula, extend the kinetic model with corresponding CHX sub-model. This is directly related to the importance of naphthene in determination of fuel combustion behavior. This was also found in the case of our previous model, where high-temperature features of the overall model were over-shadowed by HT reactions of CHX. This was particularly expected in the case of PAH productions [2, 35]. To this end, the previous published PCHX kinetic model of [36] in high-temperature ranges will be used as naphthenic sub-model instead CHX.

3. Further Development of Naphthanes Sub-model

Naphthenes are an important chemical class of hydrocarbons found in formulation of conventional fuel blends, such as diesel, kerosene and gasoline, which affects the ignition quality of the fuel. As also found in our previous researches [2, 36, 34] cycloalkanes can raise soot emission levels because they are known to dehydrogenate and produce aromatics which can initiate the chain reaction for the production of polycyclic aromatics to soot formation and growth. As already mentioned, Cyclohexane is the mostly found naphthane in various surrogate compositions, which is due to its simple structure compared with rest of the naphthane molecules. This can also benefit us to avoid complexity and reducing the model uncertainty. However, in reality the conventional fuels are made of naphthenic species that are more complex, which are in fact a combination of linear and cyclic alkanes. Due to their complex structure, their thermochemical properties, as well the combustion chemistries are rarely studied. Particularly for the larger naphthanes such as PCHX there are the matter scarce. Nevertheless, in previous works of the author the importance of substitution of PCHX within the surrogate models were discussed [36, 37]. Align with this vision, it is tried in this work to add the PCHX reaction mechanism to the recently published DSF [2] and repeat the required model development procedure to get the new surrogate composition.

The PCHX high temperature oxidation proceeds through: unimolecular fuel decomposition; H-atom abstraction leading to cycloalkyl radicals, $cyC_9H_{17}A$, $cyC_9H_{17}B$, $cyC_9H_{17}E$; β-scission decomposition; cascading dehydrogenation leading to benzene and smaller radicals; isomerization and decomposition of linear radicals after the ring-opening step. Three isomers of the cycloalkyl radicals have been included in the scheme, $cyC_9H_{17}A$, $cyC_9H_{17}B$, and $cyC_9H_{17}E$. The related rate constants were evaluated as analogous to those for the cyclohexane and propyl reactions (Fig 2).

As it can be followed from the graphic, the CHX sub-mechanism remains as the key species, which falls into decomposition through:

1) unimolecular fuel decomposition
2) H-atom abstraction leading to cycloalkyl radical, cyC_6H_{11}
3) cyC_6H_{11} β-scission decomposition, producing olefins and di-olefins
4) isomerization and decomposition reactions through ring-opening step
5, 6) cascading dehydrogenation leading to benzene and smaller radicals.

It should be noted that, all required thermochemical data were taken from Abbasi et al. 2018 [36] PCHX model, where an in-house developed tool were used to estimate the NASA-coefficients, based on the group additivity method of Benson [38]. The transport properties for PCHX intermediates are separately estimated for current study, using the group contribution methods of Joback & Reid [39] and Bosque et al. [40].
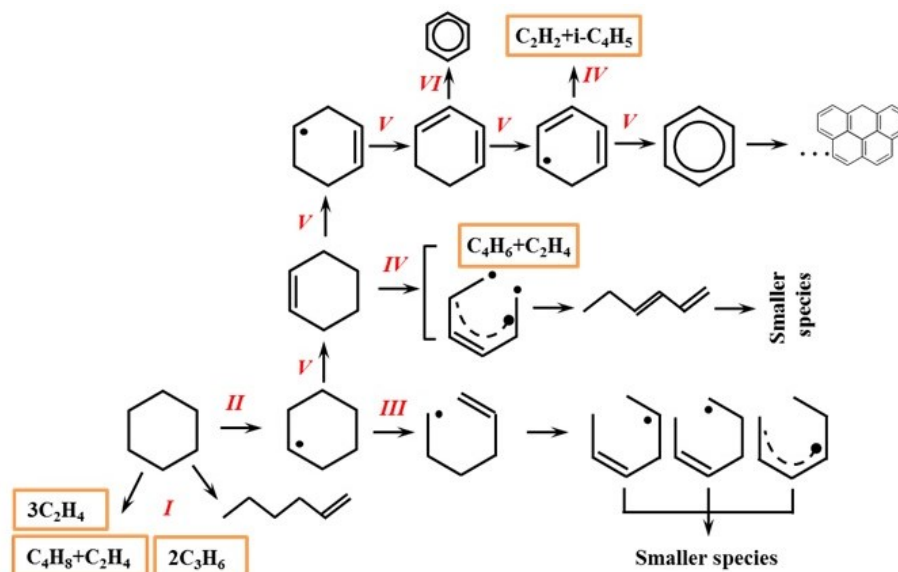
4. Adjustment of Surrogate Composition

Depending on the origin and production procedure, various fuel blends differ from each other in composition, properties (Table 1). Particularly, in the case of chemical composition, cetane number, and sulfur content, they vary strongly from each other. In our latest study [2], 3 different surrogates with different distribution of hydrocarbon classes were introduced (Fig 1), which all of them in turn could reflect the averaged physical and chemical properties of the various diesel blends. As previously spoken, SRG1 was the mostly matched surrogate in overall performance of the model withexperimental data, particularly with IDT data in LT. Therefore, it is initially tried to keep these ratios between different hydrocarbon classes and only replace CHX with PCHX (DSF-v1).

Afterwards, it is tried to improve the model response, in comparison with IDT experimental data in HT; this is done by changing the input formula, so that it can reflect the same trend as what was previously revealed. This resulted in the DSF-v2 composition (Table 3). Interestingly, the finally achieved formula is in accordance with composition of Stage V-VI diesel fuels, with no iso-alkane fraction above 20% cycloalkane content.
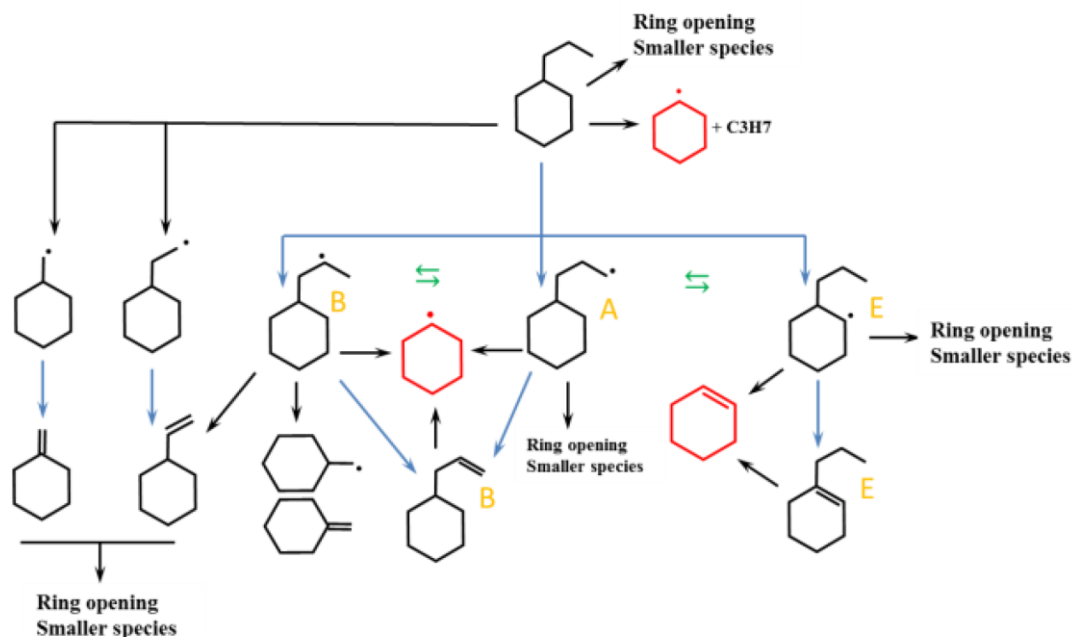
Fig 2. Principal scheme of the high temperature oxidation of PCHX [36].

Fig 3. Principal scheme of the high temperature oxidation of cyC_6H_{12} [34].

Development of a Multi-component Surrogate Model for Diesel Combustion at High Temperatures via Extension of the Naphthene Model

Table 3. The compositions of introduced surrogate compositions in this research and previous work [2].

Diesel Surrogate	Mole Fraction (%)					Averaged Formula
	C_7H_8	cyC_6H_{12}	cyC_9H_{18}	$C_{12}H_{26}$	iC_8H_{18}	
SRG1	15	20	0	50	15	$C_{9.45}H_{19.3}$
DSF-v1	15	0	20	50	15	$C_{10}H_{20.5}$
DSF-v2	35	0	25	40	0	$C_{9.5}H_{17.7}$

5. Results and discussions

The latest surrogate model was validated on a wide range of experimental data, including ST, RCM and CF data in various experimental conditions. But the recent model, developed in this research is validated against the selected experimental data, which included the LFS and IDT data in HT range (Table 4), since it contains only the PCHX chemistry in HT, and its LT chemistry is still under development.

**Table 4.** Experimental data used for model validation.

Reference	Experiment and Reactors	
	ST	CF
Haylett et al. 2009 [28]	DF/ 21% O2/ Ar P=5-7 bar, φ= 0.3-0.7 T=900-1300 K	
Gowdagiri et al. 2014 [4]	DF/ Air p=10, 20 bar, φ= 0.5, 1 T=900-1250 K	
Wang et al. 2019 [29]	DF/ Air dilution in N_2 p=6, 10, 20 bar, φ= 0.5-1 T=900-1400 K	
Chong et al. 2011 [30]		DF (ULSD-2,PME) / Air φ= 0.75-1.5, p_0= 1 atm, T_u=470 K

The diagrams of Fig 4 show the performance of the new model with both DSF-v1 and DSF-v2 against the experimental values and the response of the previous model with SRG1. The DSF-v2 composition is achieved through several iteration steps, started from setting of DSF-v1 composition as initial input formula, with the same fractions of HC classes of SRG1. These results are also included on IDT diagrams of Fig 4, which resulted in lower reactivity of model, and lower accuracy compared with experimental values, at lower operational temperatures (1000 K/T>0.85). Therefore following the trial-error procedure of surrogate modelling, yielded in a 3-component surrogate fuel of DSF-v2 at the final stage.

The simulations with newly developed surrogate model and DSF-v2 formula deliver consistent results with experimental data and within the desired uncertainty level in general. These results are very similar with what has been derived from our model (see SRG1 lines on Fig 4). This was also initially defined as one of the main goals, i.e. replacing CHX through a more realistic represent of naphthane family, without any remarkable change in the overall performance of the model in prediction of IDT data in HT ranges.

Eventually, the performance of the new model has been even improved compared with the previous model to certain extents. To get more detailed comparing both performances, the new model is more precise at higher temperatures (1000 K/T <0.8). This is particularly clear to observe at φ=1.0, P= 6-20 bar (Fig 4e,f). The accurate performance of the model on the IDT data in HT emphasises the high quality of the developed HT chemistries of surrogate model, particularly on the PCHX sub-model.

The LFS experimental data from ULSD-2 and PME biodiesel flames with synthetic air, carried by Chong et al. [30] at T_u=473 K, atmospheric pressure and φ=0.75-1.5, was also numerically investigated, implementing the current developed model with both initial (DSF-v1) and final surrogate (DSF-v2) mixtures, Fig 5. For the aim of comparison, the performance of our previous model with corresponding surrogate fuel SRG1 is also included here. As mentioned above, DSF-v1 surrogate has the same HC distribution and SRG1, although with larger averaged formula (see Table 3).
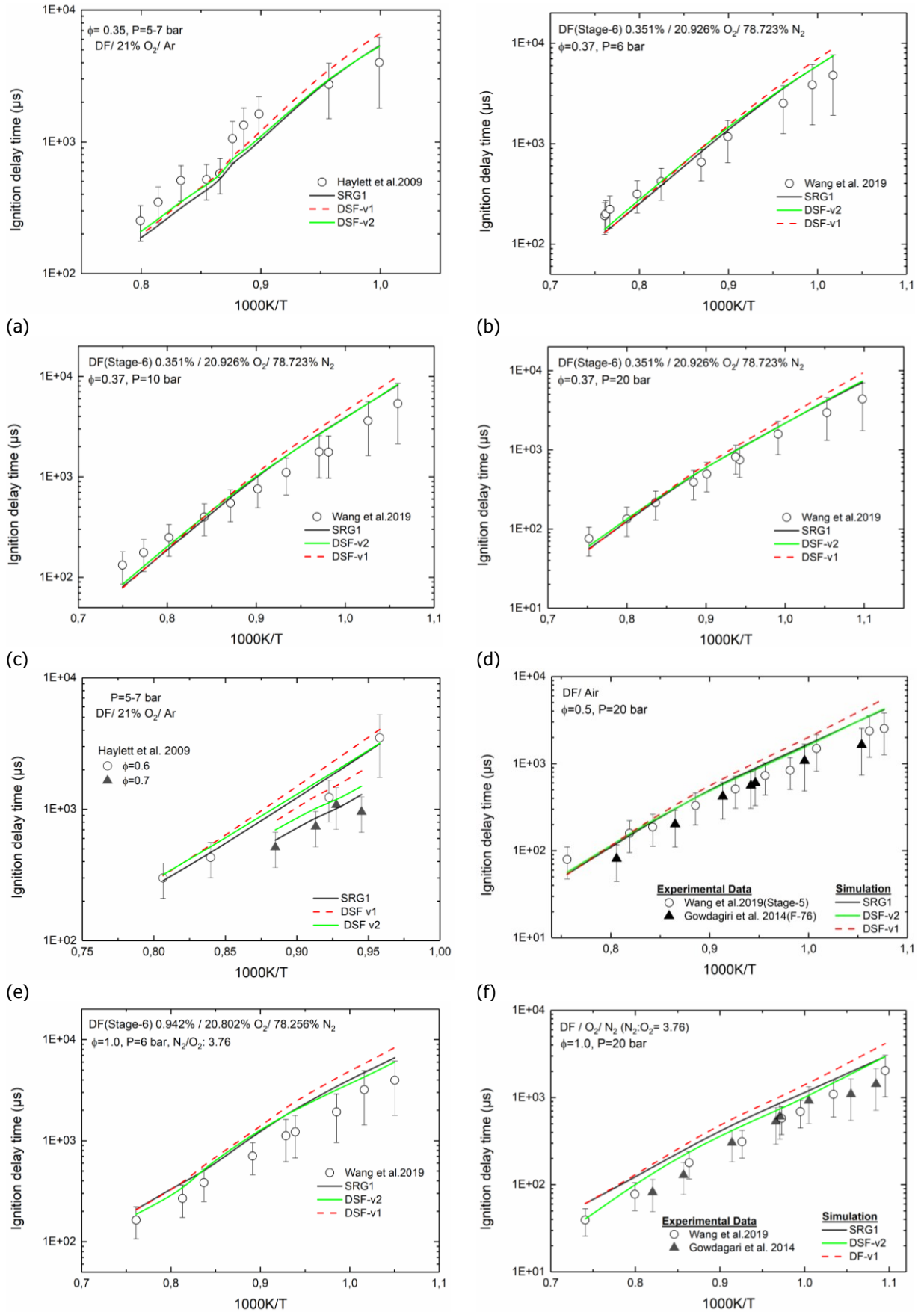
Fig 4. Simulation of experimental IDT data in HT range [4, 28, 29] with developed mechanism of present work implementing PCHX in DSF-v1,v2 compared with previous model [2] with CHX in SRG1.

Unlike the IDT data, this similarity in distribution of HC classes resulted in much closer behaviour in prediction of LFS data. However, the results from DSF-v2 mixture differ from both of them to certain extents. The DSF-v2 shows lower flame speed in φ=1.3-1.5 compared with simulations by SRG1 and DSF-v1. Moreover, the maximum flame speed is predicted to occur at φ=1.2, which is closer to the experimental data φ=1.15, but it differs slightly from simulations with SRG1 and DSF-v1, which is at φ=1.25. These differences are mainly due to the different HC composition of DSF-v2, particularly due to its higher share of naphthenic and aromatic contributions, and secondly lack of iso-alkanes (Table 3). Compared with experimental data, both models have certain level of underestimation by maximum 10 cm/s. Once can be argued that, SRG1 and DSF-v1 are closer to the experimental values in fuel-rich zone than the DSF-v2. However, if the ability in describing the data trend is taken into account, the DSF-2 is in fact more consistent with experimental data, since the steepness and curvature of experimental data are well described.
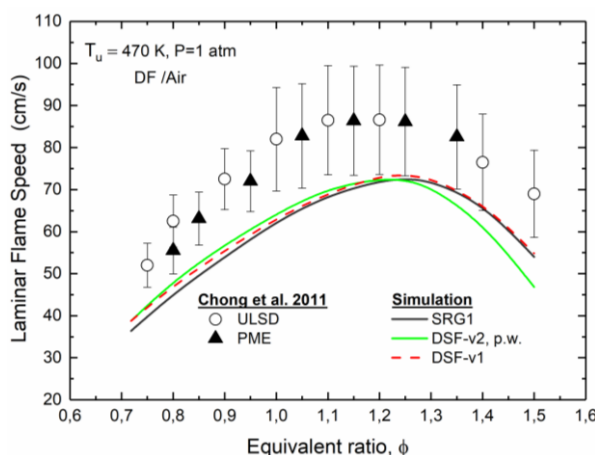
Fig 5. Simulation results of LFS data [30] through the developed surrogate model of this work, with initial (DSF-v1) and final (DSF-v2) surrogate blends, compared with previous surrogate model (SRG1) blend with CHX naphthenic basis.

6. Post-Processing of PAH Formation

The post-processing includes species rate of production ROPAD for PAH molecules, from Benzene (A1, C6H6) up to Benzo[A]Pyrene (BAPYR, C20H12) with 5 aromatic rings, which are carried via CHEMKIN PRO post processing tools [41]. Due to implemented reaction sub-models, only T>1000 K is investigated, which is from ST experiment of [29] T=1321 K, p=10 bar, φ=1.0. The ROPAD results based on the simulated results with DSM and DSF-v2 are depicted on Fig 6 for all 3 components of surrogate fuel. It is found that, similar to our previous model [2], significant fractions of large PAH molecules, such as BAPYR ($C_{20}H_{12}$) are formed directly through fuel decomposition into smaller species, which in the case of PCHX and TLN follows the ring-opening step. Afterwards, the process is mainly controlled by small chemistry C0-C3 and interactions among the corresponding species such as C_2H_3, C_2H_2, HCCO.

7. Conclusion

The recently published surrogate model for gasoil (diesel) was successfully updated on naphthenic sub-model, with the aim to include a more realistic naphthenic represent, compared with real diesel fuels. This model was originally based on the JFS model of Slavinskaya et al. [42, 43] which is then updated on C_0-C_3 chemistry by the most recent acetylene model of Slavisnkaya et al. [31], PAH sub-model of [32, 33] with ability of formation of large PAH such as BAPYR, and CHX semi-detailed kinetic model of Abbasi et al. [34].
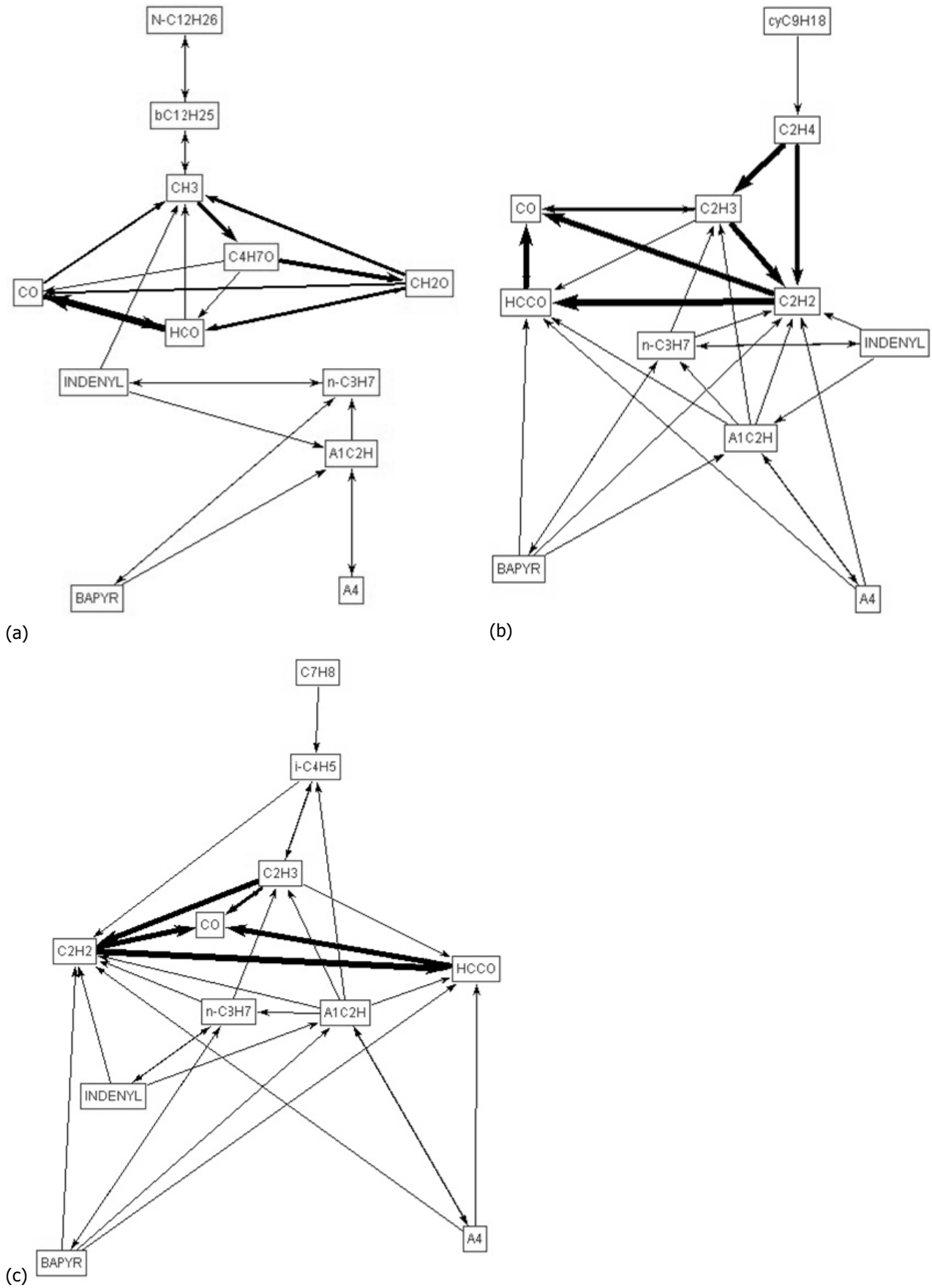
Fig. 6. ROPAD of A1 for ignition of DF/O2 at T=678 K, p=15 bar, φ=1.0, starting from each components of DSF-v2.

To this end, the formerly published HT kinetic model for PCHX [35, 36] was integrated in this model. Since the performance of the previous model was particularly successful on IDT data, the initial modeling goal is set in such a way, to successfully repeat the previous results with minimal changes. The development of the surrogate blend follows a trial-error based iterative procedure, and it begins from setting an initial IFS.

The initial fuel composition is considered similar to SRG1 in the case of HC contributions, which is selected among three previously introduced formulas (SRG1-SRG3). After certain number of iterations, the final surrogate composition is achieved (DSF-v2) which contained 35% TLN, 25% PCHX and 40% DDCN. The simulations of selected IDT and LFS data were carried through newly developed model (Fig 4,5). The initial results from DSF-v1 were also included, so that the modeling procedure and improvement of results could be tracked.

The IDT data covered T=900-1400 K, φ=0.3-1.0, and p=5-20 bar, from ST apparatuses, see Table 4. This selection of experimental data sets was due to the consideration of modeling ability in HT. As mentioned the focus of this study on HT combustion modeling of diesel. Nevertheless, the LT ignition of diesel, due to certain phenomenon occurring in this temperature ranges, such as NTC, early auto-ignition and cool flame are from high level of importance in determination of fuel characterization. In order to model the LT auto-ignition phenomenon, the kinetic model must include the LT chemistries and the corresponding intermediates properties for each HC contribution of surrogate blend. For PCHX, this remains as a matter of challenge, since there are not adequate number of studies available, focused on this issue. Even the proposed model by the authors group [35, 36] requires further theoretical and experimental investigation to ensure low level of model uncertainty. This is topic due to its importance remains as one of the future research priorities.

The simulation results provided by the model were initially closed to previous model (SRG1) for higher temperature ranges of 1000K/T <0.9. However, it deviated slightly from experimentally determined values, and also simulations with SRG1, at lower temperature at 1000 K/T >0.9 (Fig 4). Therefore, the modeling procedure continued until achievement of the mentioned initial goal, which resulted in DSF-v2 composition. The final results were in most of the cases closed to previous model, under various operational conditions. For HT ranges of 1000K/T<0.8 the new model is even more accurate than previous mechanism, compared with experimental values, see Fig 4 g, h. This proves the low model uncertainty of HT chemistries of the current model, in particular for PCHX and CHX, which was also previously concluded in [36, 35]. In recent publication of Abbasi, 2023 [2], the importance of naphthenic chemistry sub-model was particularly discussed in regards with HT chemistry and H-atom abstraction and cascading dehydrogenation. This was particularly shown by analysis of A1 formation at lower temperatures, where the cascading dehydrogenation of CHX was diagnosed as the most important working chemistry within the temperature ranges of 900-1200 K. CHX was diagnosed as one of the most probable species of PCHX dissociation at HT condition (Fig 2). The existing connection between PCHX and CHX sub-schemes (Fig 2,3) highlights again the importance of CHX chemistry in Abstraction and cascading dehydrogenation schemes in the overall kinetic model.

The prediction of LFS experimental data at T_u=470 K, atmospheric pressure, and φ=0.75-1.5 through the new model was initially (DSF-v1) similar to previous study (SRG1). After finding out the ultimate surrogate (DSF-v2), the experimental points were re-calculated, which resulted in lower speed at φ=0.3-1.5 compared with previous model. This is apparently due to the higher contents of aromatic and naphthenic compounds, and lower share of iso-alkanes in DSF-v2 compared with SRG1. However, once can conclude that they are in better agreement with experimental data, especially in prediction of the data trend, and slope of the experimentally determined curve, at both lean and rich sides. Moreover, the position of maximum flame speed is predicted at φ=1.2, which is compared to previous model better matched with experimental values. Due to the significant role of C_0-C_3 chemistries in calculation of flame speed, paying further attention to this section of the model may help us in improvement of overall model uncertainty, especially in regard with the existing underestimation, illustrated on Fig 5.

The ROPAD analysis for PAH formation was also carried at T=1321 K, p=10 bar, φ=1.0. The PAHs growth were considered until large molecules, such as BAPYR (with 5 aromatic rings) from all three components of final surrogate fuel, which were dominated by the importance of direct dissociation of the fuels into smaller species, and the C_0-C_3 chemistries throughout species such as vinyl and ketenyl radicals. This point highlight the important role of small chemistries in description of HT flame specifications.

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HiSST-2024-0073
Development of a Multi-component Surrogate Model for Diesel Combustion at High Temperatures via Extension of the Naphthene Model

Page |11
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