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**EVALUATION OF JP-8 SURROGATE UNDER SPRAY DIESEL  
CONDITIONS USING DETAILED CHEMICAL KINETIC MODELS**

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**ABSTRACT**

*Single-Fuel Concept (SFC) describes the desire to operate diesel engines using JP-8 as the only fuel in the US military due to mostly logistic reasons. However, there is a lack of a fundamental database on the combustion characteristics of JP-8 compared to those studies that have been done for diesel combustion. In this current study, several kinetic models are used to look into flame properties including ignition behavior, fuel properties including evaporation characteristics, and species evolution such as soot precursor, acetylene. Several surrogates for JP-8 fuel including tetradecane, n-dodecane and a mixture of 77 vol-% n-dodecane and 23 vol-% m-xylene are selected in the model using a detailed chemical kinetic mechanism with 330 species and 1957 reactions. Included in the model are growth mechanisms of Polycyclic Aromatic Hydrocarbon (PAH), which are known to be important for soot formation. Studies are performed to describe the fundamental combustion characteristics of JP-8 surrogates under spray diesel conditions. Numerical models used include closed reactor simulation, Two-Stage Lagrangian (TSL) model, and Computational Fluid Dynamics (CFD) simulation. Simulation conditions include temperatures range of 1000-1400 K and injection pressures of 1100 bar, and ambient density of 14.8 kg/m<sup>3</sup>. Experiment was performed with limited number of runs to compare with the result from simulation. Vapor penetration from CFD simulation currently under predicts the values from experiments.*

**INTRODUCTION**

The ease of using a single fuel in land based military aircraft, vehicle and equipment comes mainly from simplifying the fuel supply chain [1]. This has made the US Government and many research centers thrive on optimizing the performance of jet fuel, JP-8 under realistic diesel engine conditions [2-10]. In the US military, JP-5 (jet propellant-5) is used in the Navy and JP-8 (jet propellant-8) is used in the Air Force. Both fuels are colorless and have the smell of kerosene which is also the primary substance in each fuel. Similar to diesel, the combustion of JP-8 pollutant although aircrafts are known to produce significantly reduced emission compared to other type of transportation such as automobile. The carbon dioxide projection of year 2050 from aviation contribution is about 3 % of the total CO<sub>2</sub> produced by humans [11]. The current engine design is also

intended to produce more complete and rapid combustion to avoid maximum local temperature in the combustion chamber that limits NO<sub>x</sub> emissions.

While there are growing changes in policy as nation favors diesel engines over gasoline-driven equipment, the application of JP-8 fuel [12, 13] to diesel engines contains potential problems both for current and advanced combustion engines and for increased power density applications. In order to maximize efficiency while limiting smoke emissions and maintaining robust combustion for these systems when using JP-8 as a fuel, fundamental spray, ignition, and combustion properties need to be thoroughly understood and characterized. Despite the importance of these factors, fundamental databases on the combustion characteristics of JP-8 are usually rare, in compared to those readily available for diesel fuel. Consequently, the main

purpose of this study is to develop models that provide a database relevant for experimental validation.

In order to study combustion processes and eventually develop models, a blend of multiple component fuel, called a surrogate, is usually proposed to reduce the complexity of chemical reactions, and variation in fuel properties from batch to batch from realistic fuel. Three surrogates were chosen to represent JP-8 fuel including: n-dodecane, mixture of n-dodecane and m-xylene, and tetradecane. While n-dodecane and m-xylene have been used in various studies [4], tetradecane is also introduced in this study due to its higher boiling point that may better match JP-8 liquid length and vapor length behavior compared to other surrogates such as dodecane or Heptamethylnonane (HMN) [14].

Although ignition delay is one of the key parameters in the development of chemical kinetics, there has been no report focusing on the selected surrogates of this study under engine conditions. In this ignition simulation, the temperature and pressure of ambient gas were varied to characterize the effect of a wide range condition of the surrounding gas on the combustion of the fuel surrogates. Additionally, introduced in this study is the TSL [15] model that is capable of simulating spray combustion using detailed chemical kinetic mechanism. TSL is unique in permitting the inclusion of mixing processes in a computationally efficient method thereby providing continuous reactions while entrainment and other essential flow aspects are also considered [15]. Also CFD simulation will be performed to investigate the combustion phenomenon under realistic condition of the spray.

In general, the selected fuel surrogates in this study are investigated and validated using a detailed mechanism under several numerical models. This provides a preliminary results for future experiments in which information of fuel surrogate can be easily extracted such as ignition delay, liquid length, and flame propagation.

## MATERIALS AND METHODS

In this section, the mechanism, and a set of numerical approaches including closed reactor, TSL, and CFD model will be described.

### 1. Jet Surrogates

Realistic jet fuels often contain multiple components with a boiling point ranging from 160-260°C [3], jet fuel carbon number is usually ranging from 10-14. Generally, there are two common jet fuels, Jet A-1 and JP-8. JP-8 has additional requirements in military including corrosion inhibitor, icing inhibitor, and static dissipater. Jet fuel, also considered as kerosene fuel, has an average of 20% by volume n-paraffins, its surrogate usually contains large amount of n-decane, n-dodecane and n-tetradecane with less than 25% by volume aromatics and less than 3% by volume naphthalene [3].

Although single component fuel makes it simple in modeling and experimental work, it does, however, oversimplify the complexity of chemical reactions that leads to soot formation and emissions. A long-term goal in research of surrogate jet fuels is to increase number of components in a surrogate fuel while having better understanding of the kinetics of each component and with each other in chemical interaction manner. Hence, one major work in developing a surrogate fuel is to collect a fundamental database of chemical kinetics, thermodynamics, and physical properties of all species involved in the combustion reactions.

Earlier work involves matching fuel boiling range and composition [16]. This usually takes 12 component surrogates [17]. Other focuses on combustion application include various experiments such as premixed flame, stirred reactor, counterflow flame and shock tube [3]. n-dodecane showed good comparison with experimental data for liquid phases properties under wide range of temperature [18], but required complicated modeling for multi-phase behavior. Several proposed surrogates involve multiple components such as Violi [19] with six component including n-dodecane, n-tetradecane and methyl cyclohexane as the major components. Combustion Science and Energy (CSE) [20] and Reaction Engineering International (REI) [21] used only 3-4 components with majority component being n-decane. While there are many factors to consider to reduce the kinetic limitation, in the current work, three selected characteristics that were described to be high priority in surrogate evaluation. These include heat release rates, soot and particulate matter, and flame propagation based on laminar flame speed. There has been conclusion that while laminar flame speed can be matched well experimental and numerically, flame extinction can be different significantly [22]. Hence, future work will continue on study of laminar flame speed and flame extinction simultaneously of the chosen surrogate.

### 2. Mechanism Summary

One of the jet surrogates in this study contains a kinetic mechanism for n-dodecane and m-xylene blend, namely SERDP mechanism. The mechanism contains PAH chemistry. This mechanism was developed from several mechanisms including Mech II [23] for small species chemistry (less than C4 compounds), Jetsurf 1.0 chemistry for n-dodecane [24], and Battin-Leclerc model for m-xylene chemistry [25]. The final mechanism contains 330 species and 1957 reactions. However, there is no tetradecane specie involved in the SERDP mechanism. Based on a search for the mechanism of tetradecane, the oxidation mechanism for heavy n-alkanes developed by Chang et al. [26] was chosen due to its extensive validation through various experimental apparatus such as shock tube, flow reactor, counterflow

flame, premixed laminar flame, and jet-stirred reactor. This research approach involves using two mechanisms separately to study different surrogate selections. Two mechanisms were integrated to one single mechanism with soot chemistry, namely MTU. Table 1 summarizes all the mechanisms used in this study.

**Table 1:** Mechanism set summary

Mechanism	Target Surrogate	Species	Reaction	Soot Chemistry (PAH)	Source
SERDP	n-dodecane+m-xylene	330	1957	Yes	SERDP [4]
Chang	tetradecane	80	194	No	Chang [26]
MTU	n-dodecane, n-dodecane+m-xylene, tetradecane	378	2074	Yes	Combined SERDP and Chang

Using the mechanism sets mentioned above, the simulation condition is shown in table 2. This is also the condition for experimental work using a single hole injector of 100  $\mu\text{m}$  diameter size to validate model results.

### 3. Simulation Conditions

Given the objective of this study, several simulation conditions as shown in table 2. First, different mechanisms including SERDP, Chang, and MTU were compared. This is followed by the evaluation of each jet fuel surrogates: pure n-dodecane, mixture of n-dodecane and m-xylene, and tetradecane. Comparison between different models closed reactor, TSL and CFD in terms of predicting combustion behavior of jet surrogates was also performed.

The final target is to develop CFD model to predict soot and emission of tetradecane using MTU mechanism.

**Table 2:** Simulation condition summary

	Close Reactor	TSL	CFD
Fuel	n-dodecane, n-dodecane + m-xylene, tetradecane	n-dodecane, tetradecane	n-dodecane, Tetradecane
Oxidizer	15% O <sub>2</sub>	15% O <sub>2</sub>	15% O <sub>2</sub>
Phi	1	-	-
Ambient Temperature [K]	1000 -1400	1000	1000
Density [kg/m <sup>3</sup> ]	14.8	14.8	14.8, 22.8
Injection Pressure [bar]	1100	1100	1100
Nozzle diameter [ $\mu\text{m}$ ]	-	100	100

### 3a. Ignition Delay Simulation

A closed reactor model was performed to estimate the ignition delay for each surrogate over temperature range of 1000 K – 1400 K. At each ambient temperature, ambient pressure was calculated so that the ambient density was constant at 14.8 kg/m<sup>3</sup>. The two mechanism sets in this study were compared by performing ignition delay calculation using the same fuel and the same condition over the range of ambient temperature.

### 3b. TSL Simulation

Closed reactor does not include the effect of turbulent mixing which is essential in a real spray. This was improved by the introduction of TSL model, run at 1000K, injection pressure of 1100 bar, and ambient density of 14.8 kg/m<sup>3</sup>. Proper adjustment was made on the TSL model to perform spray simulation for gas-phase species. Since the TSL model was based on gas-phase simulation only, the actual jet source at the nozzle exit needs to be initialized on gas-phase fuel by matching momentum, mass flow rate, and flame temperature in order to account for approximately the same mixing rate as the liquid fuel jet. Because of fuel phase change which is required as input for the TSL simulation, the input orifice diameter is changed from its experimental input of original diameter to have the same momentum and mass flow rate for the specified ambient temperature.

### 3c. CFD Simulation

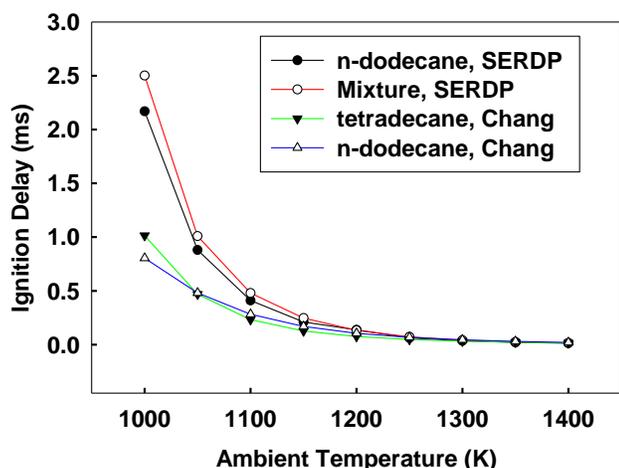
Using similar conditions as in closed reactor and TSL model, the CFD simulation with CONVERGE code [27] uses a cubical geometry representing a fixed volume combustion vessel [28], Kevin-Helmholtz (KH), Rayleigh-Taylor (RT) break-up model, and a unique combustion model with SAGE [27] detailed chemistry solver that takes into account the full input mechanism. The spray was introduced into a 10 cm x 10 cm x 10 cm cubic imitating a combustion vessel. The injection pressures are 1100 bar with 1 ms duration. In order to study the effect of ambient temperature, ambient density, and injection pressure, a number of cases were established for the CFD simulation.

## RESULTS AND DISCUSSIONS

### 1. Closed Reactor Ignition delay

Ignition delay was calculated for different surrogate selection using different mechanism as noted in the legend of figure 1 (i.e. “n-dodecane, SERDP” means using n-dodecane as fuel using SERDP mechanism). As shown in figure 1, mixture of 77% n-dodecane and 23% m-xylene give the longest ignition delay compared to pure n-dodecane and tetradecane. The ignition delay difference between of 2 component surrogates (n-dodecane + m-xylene and pure n-dodecane) using SERDP mechanism is within 0.34 ms. At

higher temperature, there is less difference in the ignition delay between each surrogate. However, there is larger difference ( $<1.36$  ms) in ignition delay when comparing the same fuel, n-dodecane, for SERDP and Chang's mechanism, implying there are certain chemical pathway distinctions between these two mechanisms that may lead difference in terms of ignition delay. Using Chang mechanism, tetradecane has less than 0.048 ms ignition delay difference than pure n-dodecane. Hence, it is concluded that there is similar trend of ignition delay for each surrogates within the same mechanism. Again, it was the objective to eventually combine two mechanisms in order to study soot and emission of tetradecane spray combustion with experimental validation.

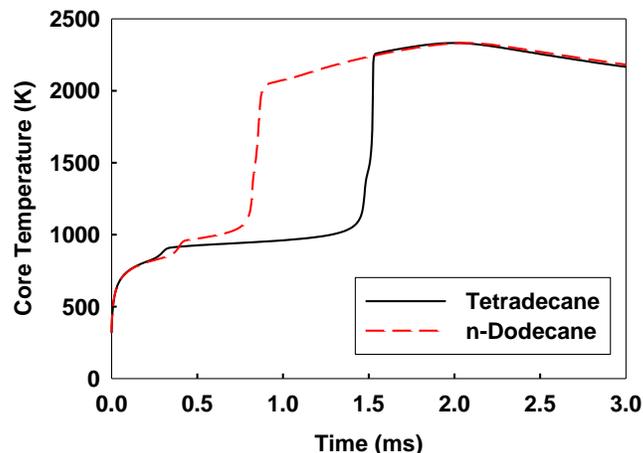


**Figure 1:** Ignition delays of different surrogates with 15%  $O_2$  mixture from closed reactor simulation at varying ambient temperature of 1000 – 1400 K using SERDP and Chang mechanism.

At temperature less 1250 K, the SERDP mechanism over-predicts the ignition delay compared to Chang mechanism while when temperature higher than 1250 K, n-dodecane reaction gives longer ignition delay in Chang mechanism. In Chang mechanism, same phenomenon occurs for two different surrogate reactions of tetradecane and n-dodecane. But the critical temperature point is 1050 K. This implies that temperature dependence needs to be considered for different surrogates in different mechanism. Further investigation to distinct the nature of these two mechanism is needed in order to obtain an integrated mechanism for soot study of the chosen surrogate. Nonetheless, the relatively small difference between ignition delays of two mechanisms gives confidence to proceed implementing soot chemistry. However, some of the species and reactions can be repetitive hence these will be disregarded in the combined mechanism.

## 2. TSL Results

The effect of mixing on ignition process was estimated by TSL mixing model. As shown in figure 2, jet core temperature of two reactions of tetradecane and n-dodecane as fuels at similar condition as mentioned in table 1.

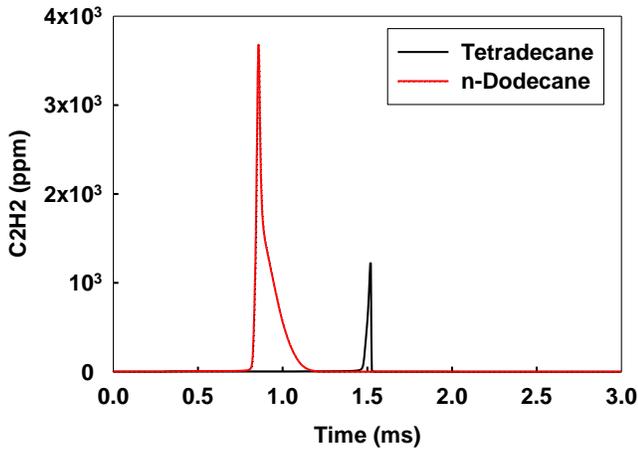


**Figure 2:** Jet core temperature of tetradecane and n-dodecane at ambient temperature of 1000K, 15%  $O_2$ , and density of  $14.8 \text{ kg/m}^3$ .

Both fuels' jet core temperature reflect the typical two-stage ignition process: first cool-flame period followed by the second-stage of the main heat release. The first stage has smaller temperature rise compared to the second-stage which has relatively fast-mixing between surrounding gas and jet core that enhance fuel oxidation. The fuel core temperature of both fuels starts at 300 K. The ignition delay is defined as the duration between when jet core reach ambient temperature (1000 K) and the point where maximum temperature gradient occurs. The ignition delay for tetradecane and n-dodecane are 0.21 ms and 0.18 ms, respectively.

The growth of polycyclic aromatic hydrocarbon (PAH) species is characterized by the hydrogen abstraction carbon additions (HACA) mechanism up to seven-ring PAH molecules and large gas-phase PAH molecules are used as an indication for subsequent soot formation. Kitamura et al. [29] stated that pyrene ( $C_{16}H_{10}$ ) is the four benzene-ring PAH to represent soot precursor sufficiently. Pyrene is a large gas-phase PAH representative of soot precursor while the formation of acetylene followed by benzene is also considered since these are important species that lead to the formation of pyrene. Unfortunately, Chang mechanism does not include benzene and pyrene, hence, the profile of acetylene was considered as shown in figure 3.  $C_2H_2$  peak concentrations are at 0.9 ms and 1.5 ms for n-dodecane and tetradecane respectively. The late production of  $C_2H_2$  in

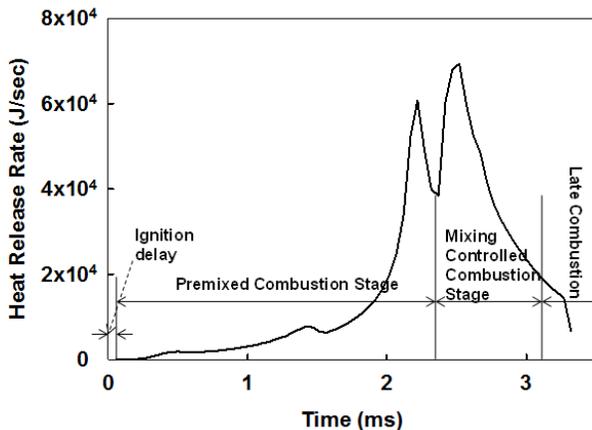
tetradecane could be caused by the larger number of carbon to be broken in the fuel,  $C_{14}H_{30}$ , compared to n-dodecane ( $C_{12}H_{26}$ ).



**Figure 3:**  $C_2H_2$  mole fraction from reactions of fuel tetradecane and n-dodecane at ambient temperature of 1000K, 15%  $O_2$ , and density of  $14.8 \text{ kg/m}^3$  using Chang mechanism.

### 3. CFD Results

The overall compression-ignition diesel combustion process can be seen in the CFD result as shown in figure 4. The ignition delay of n-dodecane using Chang mechanism was found to be approximately 0.1 ms, and premixed combustion lasts about 2.3 ms.

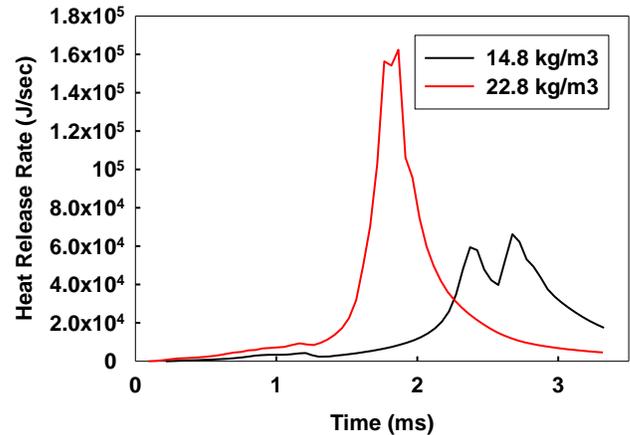


**Figure 4:** Heat release rate of n-dodecane combustion in 15%  $O_2$ , 1000 K, 1100 bar injection pressure,  $100 \mu\text{m}$  nozzle diameter,  $14.8 \text{ kg/m}^3$  ambient density.

The reaction of n-dodecane was also performed for SERDP and MTU mechanisms. However, the value of ignition delay was not reasonable: 2.2 sec (SERDP) and 0.55 ms (MTU). Currently, the CFD simulation focused on using

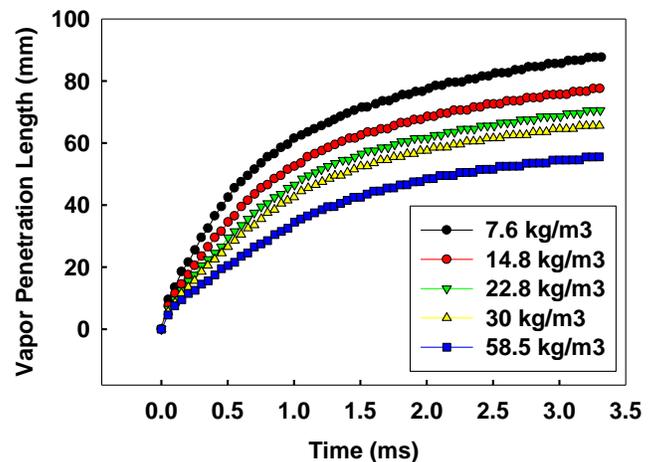
Chang mechanism which contains a relatively small number of species and reactions for ease of computation.

At different ambient densities, the heat release rate of tetradecane, the selected jet surrogate fuel, is shown in figure 5 as function of time. The ignition delay is 0.1ms and 0.25 ms, respectively, for  $22.8 \text{ kg/m}^3$  and  $14.8 \text{ kg/m}^3$  cases.



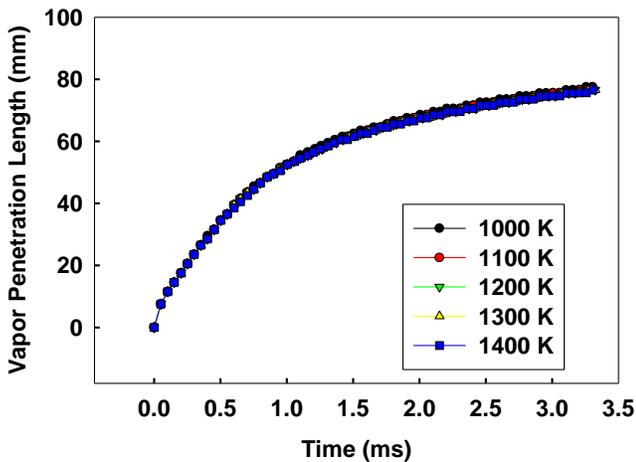
**Figure 5:** Heat release rate of tetradecane combustion in 15%  $O_2$ , 1000 K, 1100 bar injection pressure,  $100 \mu\text{m}$  nozzle diameter at two different density,  $14.8$  and  $22.8 \text{ kg/m}^3$ .

The effect of different ambient densities on vapor penetration length is shown in figure 6. As expected when increasing the ambient density, vapor penetration decreases. The change in vapor penetration is noticeable immediately after the start of injection, i.e.,  $ASOI=0$  sec. Faster vapor penetration also results in longer liquid vapor penetration for low ambient density cases.

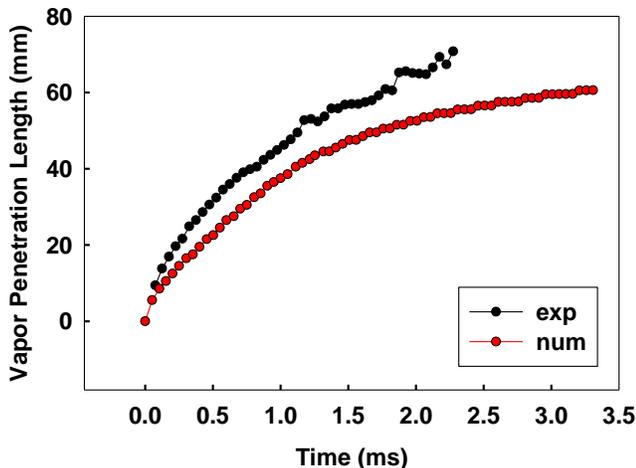


**Figure 6:** Penetration length at different ambient density at 1000 K ambient temperature, 1100 bar injection pressure,  $100 \mu\text{m}$  nozzle diameter.

There is no change in vapor penetration in the study of ambient temperature as shown in figure 7. As the temperature increase from 1000 K to 1400 K, vapor penetration decreases by maximum of 3.4 %. This is similar result observed in the experimental part of this study [29]. However, the effect of temperature on vapor penetration is expected since the ambient density was constant leading to nearly constant air entrainment for the same amount of fuel injected into the control volume environment. Further investigation is necessary on the temperature impact on the vapor penetration.



**Figure 7:** Penetration length at different ambient temperature of 1100 bar injection pressure, 15% O<sub>2</sub>, 14.8 kg/m<sup>3</sup> ambient density, 100 μm injector diameter.



**Figure 8:** Penetration length comparison for single injection with injection pressure of 700 bar, ambient temperature of

1080 K, ambient density of 25.7 kg/m<sup>3</sup>, 0% O<sub>2</sub>, nozzle diameter of 100 μm.

Only a limited number of experimental data was obtained in this study [30]. One result was compared with the CFD simulation as shown in figure 8. The numerical under-predicts the collected vapor penetration length. Several model constants such as diffusivity constant of the evaporating species, tetradecane, should be considered in the simulation. This lead to future refinement in the modeling work to match fuel properties and the physic of spray. Additional, it is important that a number of repetitive experiments is needed to characterize the fuel penetration at a given condition.

### SUMMARY AND FUTURE WORK

Several jet surrogates were selected in this numerical study of ignition delay using closed reactor, TSL, and CFD model. Key findings from this work include:

- Chang mechanism with jet surrogate fuel as tetradecane provide good representation of combustion behavior basing on the results of TSL and CFD. This is a good application in further investigating the surrogate under a wide range of diesel combustion condition. Additionally, the computation requires less amount of time due to small number of species and reactions in the mechanism.
- At temperatures below 1250 K, Chang mechanism has shorter ignition delay compared to SERDP mechanism with n-dodecane as fuel. As temperature increases above 1250 K, Chang mechanism predicts longer ignition delay.
- Mixture of n-dodecane and m-xylene is less than 15% different in ignition delay compared to pure n-dodecane using SERD mechanism.
- n-dodecane produces soot precursor (C<sub>2</sub>H<sub>2</sub>) earlier than the reaction of tetradecane at 15% O<sub>2</sub> ambient condition.
- Increasing ambient density results in the reduction of vapor penetration.
- Ambient temperature from 1000 K to 1400 K has nearly no effect on vapor penetration in the CFD simulation.
- Vapor penetration is shorter in the model compared to a single experimental data with average of 10 % in penetration length.

### Future work

- The difference of ignition delay between SERDP and Chang mechanisms for the same condition of fuel and other conditions, indicates that more

detailed study of the chemical kinetics of these two mechanisms is needed. This also provides more insights to modify MTU mechanism in order to investigate soot and emission of tetradecane combustion.

- Heat release rate was able to extract ignition delay information of tetradecane and n-dodecane using Chang mechanism. The results are relatively reasonable but require further validation through experiment.
- Extending numerical study in laminar flame speed and flame extinction can benefit the validation of MTU mechanism with the original mechanisms from SERDP and Chang.
- Other soot precursors such as benzene and soot indicator (pyrene) can be extracted once MTU mechanism is validated. The combination of CFD and detailed chemistry will potentially provide accurate simulation of engine performance.
- Further experiment is needed to provide an exclusive database for simulation validation at various conditions of spray.

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