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## A Compact Naval Fuel Kinetic Model for Marine Diesel Engine Combustion

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# A Compact Naval Fuel Kinetic Model for Marine Diesel Engine Combustion

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**Abstract.** In this study, a compact multi-component kinetic model with 129 species is used as a surrogate model to represent the actual naval fuel, namely F-76. The surrogate fuel compositions are determined according to the actual fuel compositions of F-76. Subsequently, the model is comprehensively validated in zero-dimensional chemical kinetic simulations under a wide range of shock tube and jet-stirred reactor conditions. Good agreement between the reduced and detailed model is achieved for ignition delay and species profile predictions, with a maximum deviation maintained to within 40%. The surrogate model has demonstrated a satisfactory compromise between model accuracy and kinetic size.

## 1. Introduction

To date, the conventional compression-ignition diesel engines are still widely used as the main propulsion system in the marine sector for its reliability as well as fuel efficiency. Nonetheless, it is inevitable that various green-house emissions are generated as result of the naval fuel combustion in the marine diesel engine, such as carbon dioxide (C), methane (M), nitrous oxide, carbon monoxide, non-methane volatile organic compounds (NMVOCs) and sulphur dioxide (S). In view of this, development of more efficient engines as well as cleaner fuels are essential. In order to achieve this target, a better understanding on the combustion and pollutant formation events for the naval fuel combustion is imperative. In general, numerical modelling approach is preferred for these investigation studies as it is found to be more cost-efficient in comparison to the experimental approach. Therefore, the Computational Fluid Dynamic (CFD) simulation, is adopted in this study which encompasses two major phases: (1) selection of naval fuel kinetic model for marine diesel engine combustion, (2) model validation under marine diesel engine conditions. The kinetic model applied here is expected to mimic the combustion behaviors of actual naval fuels, namely F-76.

It is noted that different combinations of fuel surrogate component are desired in order to replicate the exact compositions of the actual naval fuel so that better agreement in the fuel kinetic performance and pollutant formation can be achieved. However, most of the kinetic models only consists of selected fuel components from the hydrocarbon families (e.g. straight-chain hydrocarbons). On top of these, it is also found that mechanisms with long-carbon-chain structures are more suitable to represent the complex naval fuel chemistry. Set against this background, this work aims to investigate the application of a multi-component long-chain kinetic model as a surrogate model for F-76. The model compositions are adjusted according to those of F-76. Subsequently, it will be validated in zero-dimensional (0-D) kinetic simulations under both auto-ignition and jet-stirred reactor (JSR) conditions.



## 2. Properties of Naval Fuel F-76

F-76 is a naval fuel which is commonly used in marine compression-ignition engines, naval gas turbines and ship boilers. The main fuel constituents of F-76 are including 59.88% n-alkane, 25.38% iso-alkane, 4.73% naphthene, 7.23% aromatics, 1.52% tetralin and 1.26% olefins [1]. The physical properties of F-76 are provided in Table 1. In this work, a compact kinetic model comprising four different fuel components, such as aromatics, straight-, branched-, and cyclo-alkanes, is applied as the surrogate model to emulate the combustion behaviours of the naval fuel F-76 under marine diesel engine-like conditions. It is worth-mentioning that the compositions of tetralin and olefins in the actual fuel are relatively low and hence their kinetic reactions are not considered in this study. The details of the surrogate model are depicted in Table 2. n-Hexadecane (HXN), 2,2,4,4,6,8,8-heptamethylnonane (HMN), cyclohexane (CHX) and toluene are the representatives of straight-alkane, iso-alkane, naphthene and aromatics, respectively. The corresponding composition of each fuel component is determined according to the actual fuel compositions. Further details of the compact surrogate model can be found in [2].

**Table 1.** Physical Properties of F-76 [1].

Properties	Values
Compositions (%):	
n-Alkane	59.88
iso-Alkane	25.38
Naphthene	4.73
Aromatics	7.23
Tetralin	1.52
Olefins	1.26
Density (g/ml)	0.845
Viscosity (cSt)	3
LHV (MJ/kg)	42.6
H/C ratio	1.8249
CN	51

**Table 2.** Details of surrogate model.

Properties	Values
Compositions (%):	
n-Alkane	60
iso-Alkane	26
Naphthene	5
Aromatics	9
Model size:	
No. of species	129
No. of reactions	411

## 3. 0-D Kinetic Simulations

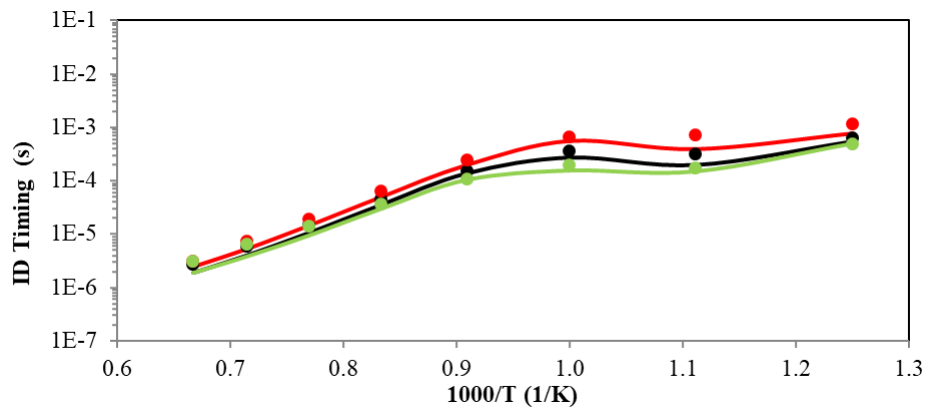
In this study, a FORTRAN-based chemical kinetics package, i.e. CHEMKIN-PRO, is utilized to compute the gas- phase reactions involved in 0-D closed reactor systems. Here, a 0-D closed homogeneous batch reactor and an open perfectly- stirred reactor (PSR) models are applied throughout the kinetic studies. The closed homogeneous batch reactor is used to simulate dynamic reactor conditions in which the controlling conditions vary with respect to time. The ignition delay (ID) timings predicted by the surrogate model in a constant volume system along with the key species profiles are calculated as a function of time. On the other hand, the open PSR model, is used to simulate steady-state reactor systems from which species profiles as a function of ambient temperature are computed. The operating conditions for the 0-D simulations are presented in Table 3. The operating conditions are chosen based on the typical in-cylinder parameters for marine diesel engine.

**Table 3.** Operating conditions of the 0-D kinetic simulations.

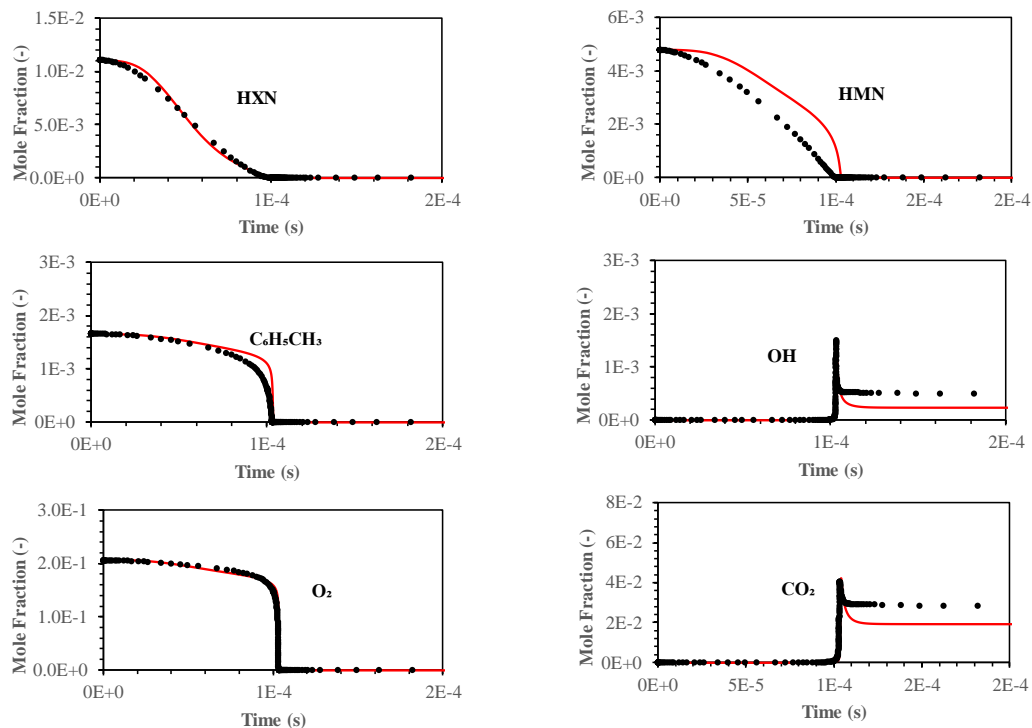
Parameters	Values
Auto-ignition Condition	Pressure (bar)
	80, 100, 120
	Temperature (K)
JSR Condition	800 - 1500
	Equivalence ratio, $\Phi$ (-)
	0.5, 1, 2
	Pressure (bar)
JSR Condition	80, 100, 120
	Temperature (K)
	800 - 1500
JSR Condition	Residence time (s)
	1

#### 4. Results and Discussions

In this section, the predicted results by the compact surrogate model are compared with the computations of its detailed counterpart using the operating conditions depicted in Table 3. This is to ensure that the kinetics of the detailed model are reasonably represented by the compact surrogate model. First and foremost, the calculated IDs by the reduced and detailed models under auto-ignition conditions are compared, as shown in Figure 1. Only results for pressure of 80 bar are presented as the predicted ID trends are comparable with those for initial pressures of 100 bar and 120 bar. Based on the results demonstrated in Figure 1, it can be observed that the ID timing predictions for the compact surrogate model agree closely with those of its corresponding detailed counterpart throughout the parameter range.

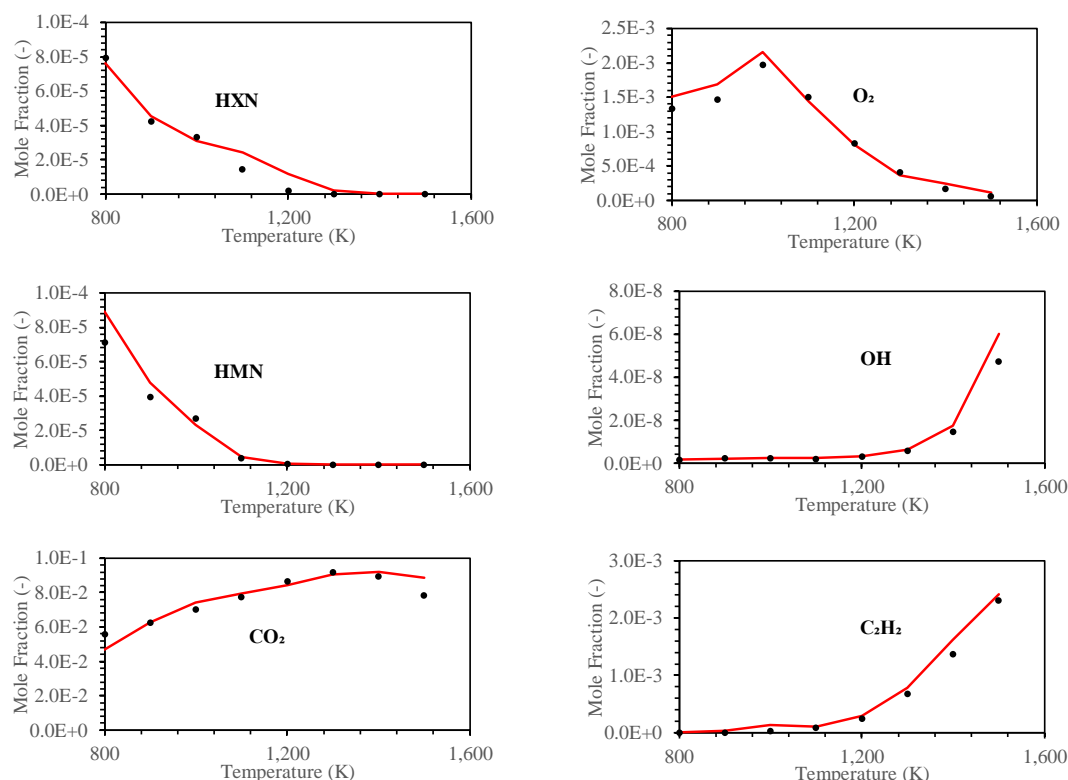


**Figure 1.** Comparisons of the ID predicted by the reduced and detailed models for initial pressure of 80 bar, and  $\Phi$  of 0.5 (red), 1 (black) and 2 (green).



**Figure 2.** Computed species profiles by the reduced (lines) and detailed (symbols) models under auto-ignition condition, with initial pressure of 80 bar, initial temperature of 1100 K and  $\Phi$  of 2.

On the other hand, capability of the surrogate model in reproducing the concentration of important combustion reactants/products is also examined. Comparisons of the reduced and detailed models with respect to species concentration profiles for auto-ignition as well as JSR conditions are shown in Figures 2 and 3, respectively. Only results for initial pressure of 80 bar and  $\Phi$  of 2 are presented since similar temporal evolution trends in the results are observed for other conditions.



**Figure 3.** Computed species profiles of fuel oxidations by the reduced (lines) and detailed (symbols) model under JSR condition as a function of temperature, with initial pressure of 80 bar and  $\Phi$  of 2.

Referring to Figures 2 and 3, it is observed that trends of the species concentration profiles computed by the detailed model for both auto-ignition and JSR conditions are retained when using the compact surrogate model. A small deviation is obtained between the computations of the reduced and detailed models. This may be partly due to the elimination of isomers in the reduced model during the mechanism reduction process. However, the results obtained here are deemed acceptable as a compromise between kinetic size and results accuracy.

## 5. Conclusions

In this study, a compact chemical kinetic model with 129 species is employed as a surrogate model for the actual naval fuel, namely F-76, under marine diesel engine-like operating conditions. The compact surrogate model is well-validated under both auto-ignition and JSR conditions. In overall, all the ID timings and species concentration predictions by the compact surrogate model are in good agreements with those calculated by the detailed counterpart. The maximum deviations from the detailed model are retained to within 40 % throughout the test conditions. The model applied in this study has shown to be able to predict the fuel reactivities reasonably well. Nonetheless, investigation on the ignition and emission characteristics of the surrogate model under non-reacting/reacting fuel

spray conditions is necessary to assess its fidelity in spray combustion computations, which will be the subject of future work.

### Acknowledgements

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### References

- [1] Reitz R, Ghandhi J, Ra Y, Rothamer D, Rutland C, Sanders S, et al. 2013 Development of Assessment Methods for Alternative Fuels for Naval Diesel Engines.
- [2] Poon H M, Pang K M, Ng H K, Gan S and Schramm J 2016 Development of multi-component diesel surrogate fuel models – Part II: Validation of the integrated mechanisms in 0-D kinetic and 2-D CFD spray combustion simulations *Fuel* **181** 120.
- [3] Poon H M 2016 Development of integrated chemical kinetic mechanism reduction scheme for diesel and biodiesel fuel surrogates for multi-dimensional CFD applications *Thesis* University of Nottingham.