

CONSTRUCTION AND VALIDATION OF A REDUCED MECHANISM IN A DIESEL ENGINE FUELED WITH 2-METHYLFURAN-DIESEL

by

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The addition of 2-methylfuran into diesel has been studied extensively to deal with the fossil energy crisis and reduce pollutant emissions. However, the chemical reaction mechanism of the engine combustion model related to 2-methylfuran is rarely reported. In this study, a reduced 2-methylfuran chemical reaction mechanism was developed by the directed relation graph with error propagation, reaction path analysis, sensitivity analysis and rate of production analysis. Then it was coupled with a diesel mechanism, and the pre-exponential factor A of the Arrhenius equation was adjusted for specific reactions to finally form a reduced 2-methylfuran-diesel mechanism containing 55 species and 190 reactions for application in combustion modelling under engine related conditions. Based on the experimental data in the literature, the predicted ignition delay time and species mole fractions by the mechanism were validated. Also, the 3-D simulation data was compared with the test data of cylinder pressure and heat release rate from a single-cylinder diesel engine under different working conditions. The simulation results of the mechanism with certain stability and accuracy are basically consistent with the experimental data and can be used to analyze the characteristics of 2-methylfuran-diesel combustion on Diesel engines.

Key words: 2-methylfuran, diesel, mechanism, Diesel engine

Introduction

The dependence of the internal combustion engine on fossil fuels brings various problems. Moreover, the fossil energy crisis and the increasing air pollution drive the mankind to seek new RES. For these two reasons, biofuels with low pollution emissions and renewability have become an important choice. The 2-methylfuran (MF) is produced by hydrogenation of furfural at 170 °C under the catalysis of copper, which is suitable for mass production and does not affect grain output [1]. The addition of oxygenated fuel has a certain effect on reducing soot emissions during diesel combustion [2]. The MF has larger octane number and higher knock resistance than gasoline. Compared with ethanol fuel, MF has lower vaporization latent heat and higher calorific value, which can significantly improve the ignition behavior. Moreover, MF has a lower cetane number and longer ignition delay time than diesel, which makes the mixed fuel more uniform in the cylinder [3, 4].

The MF has been mixed into fossil fuels to improve engine and combustion performances and reduce pollutant emissions of Diesel engines. Diesel fuel mixed with MF has more oxygen

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molecules, longer ignition delay time, faster evaporation and more uniform mixture formation ratio than pure diesel fuel [5]. Wang *et al.* [6] studied and measured the emissions of CO, NO_x, HC, particulate matter and aldehydes (formaldehyde and acetaldehyde) from MF on a single-cylinder direct injection spark ignition engine. Under 8.5 bar IMEP, the HC emission of MF was 40% and 73% lower than those of DMF and gasoline, respectively. At 6.5 bar IMEP, the formaldehyde emission from MF was the lowest among the tested fuels. Compared with gasoline, the number of particles in MF decreased by 57.9% in the nucleation state and by 238% in the accumulation state. However, under 3.5 bar IMEP, MF emitted 82%, 281%, and 40% more NO_x than gasoline, ethanol and 2,5-dimethylfuran (DMF), respectively. Katuska [7] described the characteristics of soot formation during combustion of diesel blended with MF or DMF and found that the reduction of soot emission from the diesel engine was due to different factors when using a diesel/furan derivative mixture, such as operating conditions, and combustion characteristics and physiochemical properties of the fuel. Xiao *et al.* [8] showed that when the pre-injection ratio was 20%, HC and CO emissions were greatly reduced, but NO_x emissions increased after MF was added into the pre-injection fuel. The exhaust gas re-circulation technology can effectively reduce NO_x emissions. Liu *et al.* [9] studied the effects of engine control parameters such as ignition advance angle, air-fuel ratio, injection advance angle and injection pressure on MF in-cylinder combustion and engine performance under typical medium and high loads with gasoline and ethanol as controls. The results showed that at medium and high loads, MF is more robust to lean combustion than gasoline and ethanol, and the combustion characteristics and heat release rate of MF are less sensitive to the change of injection time. Hoanga [5] found MF/fossil fuel blends with an MF ratio less than 20% were suitable for both Diesel and gasoline engines.

In recent years, researchers have extensively studied the foundational combustion characteristics of MF and constructed a detailed chemical reaction mechanism. Sirjean *et al.* [10] and Lifshitz *et al.* [11] established a detailed DMF chemical reaction mechanism, including the decomposition process of important primary and secondary products, such as cyclohexanone, MF, furan, phenol, cyclopentadiene and vinyl acetylene. This mechanism was verified by comparing with the measured results of the ignition delay time of the shock tube and the distribution of temperature decomposition products. Based on the DMF combustion kinetic model, Tran *et al.* [12] improved the furan mechanism and hydrogen atom addition process and developed a three-component chemical reaction mechanism including furan, MF and DMF. The new mechanism verified in detail the relationships of the mole fractions of reactants, products, stable and active intermediates with the flame distance of the burner [13, 14]. Tian *et al.* [15] developed a furan chemical reaction mechanism containing 206 species and 1368 reactions, which can accurately fit the mole concentration distribution of species at low pressure (35 Torr) with premixed laminar furan / oxygen/AR flame at equivalence ratios of 1.4, 1.8 and 2.2. Tay *et al.* [16] reduced the detailed chemical reaction mechanism constructed by Somers to 545 species and 2768 reactions. Based on the skeleton oxidation mechanism of the diesel alternative fuel model constructed by Chang *et al.* [17], a four-component chemical reaction mechanism consisting of furan, MF, DMF, and toluene was established, with 62 species and 228 reactions. All furan species in this mechanism were verified by the simulated and experimental data of the ignition delay time and component concentration distribution, and its moderate accuracy and stability were proved by results [16-20].

At present, MF is mainly used in combination with fossil fuels, but the reaction mechanism of MF-diesel is rarely reported. Therefore, this study aims to construct a chemical reaction mechanism of MF-diesel suitable for engine numerical simulation. Then the mechanism is verified by experimental data such as ignition delay, laminar flame component concentration

and engine cylinder pressure. It is expected that the mechanism can accurately simulate the aforementioned data and be used in engine numerical simulation reduce the simulation cost.

Construction of MF-diesel reduced mechanism

Reduced chemical reaction mechanism of MF

The detailed chemical reaction mechanism developed by Tran *et al.* [12] was selected here, which includes 305 species and 1472 reactions. This mechanism describes the reaction processes of three species viz. furan, MF and DMF under low pressure premixed flame conditions in detail. The MF reaction partially verifies the molar concentration distribution of more than 60 species and can accurately predict the flame structure.

The basic mechanism was reduced using methods such as directed relation graph with error propagation (DRGEP), reaction path analysis (RPA), sensitivity analysis (SA), and rate of production analysis (ROP). There are four main reduced steps include:

- The relevant species and reactions of furan and DMF in the basic mechanism are deleted to only retain the MF Part.
- The retained MF portion is further reduced by DRGEP to remove the species and reactions with low correlation. The threshold of error is set to 30%. The non-important species and reactions are removed step-by-step by iteratively comparing the ignition delay errors between the original mechanism and the initial reduced mechanism. In this process, the error cannot exceed the user-set value.
- The RPA, SA and ROP are used to further simplify the obtained new mechanism and retain the more important part.
- Isomers merged to reduce the number of species and adjust the mechanism.

Finally, an MF reduced mechanism containing 44 species and 169 reactions is obtained. As shown in fig. 1, MF mainly generates two products at 1000 and 1400 K. The principal one is furylCH_2 , which is mostly formed via H-abstractions by HO_2 and OH radicals. The secondary one is furan from the break of C-C between C_4 and methyl radical. Once formed, furylCH_2 almost entirely causes C_4H_5 and CO to undergo ring-opening reaction at C-O between O and C_4 atom, H-transfer from C_1 to C_4 , and C-C broken between C_1 and C_2 at both 1000 and 1400 K. The followed cracking reaction of C_4H_5 forms C_2H_3 and C_2H_2 . After that, the reaction of C_2H_3 with O_2 produces HCO and CH_2O or CO and CH_2O . Among them, HCO and CH_2O lead to CO under further reactions. Noticeably, the reaction rate of C_2H_3 with O_2 decreases obviously with the temperature rise from 1000 to 1400 K.

Furan can hardly react further to form furyl-2 . Once furyl-2 is formed, however, it almost forms CO through ring-opening reaction at C-O

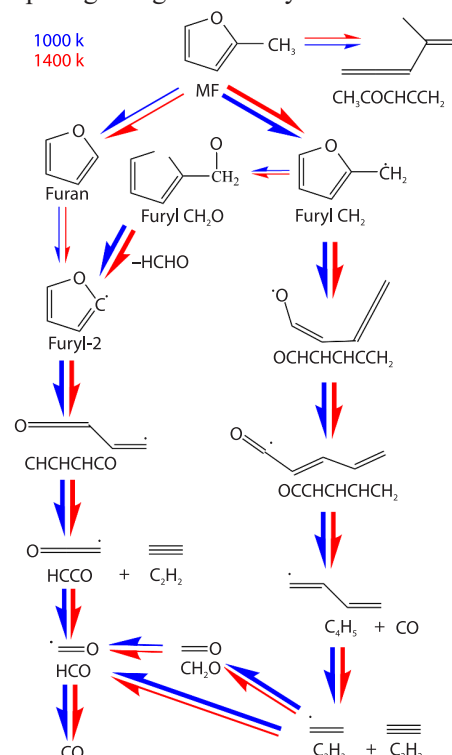


Figure 1. Main reaction pathways of MF at $\phi = 1.0$ and 5 atm. Red arrows represent the important high temperature reactions; blue arrows represent the important low temperature reactions

between O and C₄, C-C breakage in CHCHCHCO and HCCO, and H-abstraction of HCO at both 1000 and 1400 K.

Chemical reaction mechanism of diesel

The *N*-heptane is widely verified as a surrogate fuel for diesel [21]. Hence, the diesel mechanism is based on the *n*-heptane reaction in the reduced TRF-RAH mechanism constructed by Li *et al.* [22]. This mechanism was verified by shock tube ignition delay, product mole fraction distribution and engine test. Results show this mechanism can accurately predict the combustion development process of diesel in the engine. Chang *et al.* [17] proposed that the ignition process from low to high temperature can be well reproduced by optimizing the rate constants of fuel-specific reactions and keeping the reactions in the H₂/CO/C₁-C₄ system to *n*-alkanes, isoalkanes, cycloalkanes and aromatic hydrocarbons unchanged. The C₂-C₃ and H₂/CO/C₁ reactions constructed by Chang *et al.* [17] were added to the *n*-heptane reaction describe the oxidation process of small molecules. Finally, a reduced diesel mechanism containing 44 species and 167 reactions was obtained. The mechanism was verified by the ignition delay time of shock tube, laminar flame velocity and laminar flame species mole fraction distribution, and the simulation value can accurately fit the experimental value.

Construction of MF-diesel reaction mechanism

The diesel mechanism constructed in the previous step was selected as the basic mechanism, and was coupled with the reduced MF mechanism to form an MF-diesel combined mechanism. However, since the small species reactions in MF were deleted, the pre-exponential factor *A* of the Arrhenius equation shall be adjusted for specific reactions in the combined mechanism to better fit the test data. Several reactions that greatly influence MF ignition delay were obtained through sensitivity analysis. At high temperature (1400 K), the decomposition reaction of MF, shown as R1 in tab. 1, has the greatest impact on the ignition delay. This is because the reaction is competitive with reaction R3. The progress of R3 consumes a large amount of OH, and the OH concentration is an important factor affecting the ignition delay. Therefore, reaction R1 reduces the MF concentration and inhibits reaction R3, which restricts the reduction of OH concentration. At low temperature (1000 K), reaction R4 will generate abundant H₂O₂, and the increase of H₂O₂ concentration will significantly promote the positive progress of reaction R8, rapidly increasing OH concentration and releasing much heat. Therefore, reaction R4 is crucial to the ignition behavior in the low temperature region. The main reactions of MF at low and high temperatures and the adjustment of its pre-exponential factor *A* are shown in tab. 1.

Table 1. The MF main reaction and regulation of preexponential factor *A*

Major reaction pathways	Optimized <i>A_i</i>	Original <i>A_i</i>
R1 MF = CH ₃ COCHCCH ₂	6.04 · 10 ⁵⁷	6.04 · 10 ⁵⁸
R2 MF + H = furan + CH ₃	—	7.00 · 10 ⁴
R3 MF + OH = furylCH ₂ + H ₂ O	—	5.10 · 10 ³
R4 MF + HO ₂ = furylCH ₂ + H ₂ O ₂	0.95 · 10 ⁶	0.90 · 10 ⁴
R5 CH ₃ CO+C ₃ H ₃ =CH ₃ COCHCCH ₂	4.04 · 10 ¹¹	4.04 · 10 ¹⁵
R6 furylCH ₂ =OCHCHCHCCH ₂	2.05 · 10 ¹⁴	2.05 · 10 ¹³
R7 OCHCHCHCCH ₂ =OCCHCHCHCH ₂	5.7 · 10 ¹⁴	5.70 · 10 ¹⁰
R8 H ₂ O ₂ (+M)=OH+OH(+M)	—	2.00 · 10 ¹²

Through the aforementioned method, a highly compact MF-diesel simplified mechanism was obtained, which contained 55 species and 190 reactions. Although these reduced methods may bring some uncertainties to the mechanism, they will greatly reduce the cost of engine numerical simulation. In the future, we will further optimize the mechanism to improve its stability and accuracy in practical application.

Reduced MF-diesel mechanism verification

Ignition delay verification

Since the combined mechanism integrates the MF reduced mechanism and the diesel reduced mechanism and to ensure the reliability and stability of the combined mechanism, we shall verify its ignition delay. The whole ignition delay was simulated in a closed homogeneous combustion model on Chemkin-Pro. Ignition delay time is defined as the time interval for the temperature rise of 400 K from the initial unburned gas temperature.

Figure 2 compares the simulated values by the MF-diesel reduced mechanism with experimental values of the ignition delay time of *n*-heptane measured by Ciezki *et al.* [23] and Hartmann *et al.* [24] in the shock tube. When the equivalent ratio is 1 (or 2), the pressure is set to 13.5 bar and 40 bar (or 13.5 and 42 bar). The temperature range is 600-1500 K. The simulated *n*-heptane ignition delay curve of the combined mechanism well agrees with the experimental curve in both low and high temperature zones. When the temperature is low, the influence of pressures on the ignition delay is relatively small. The combined mechanism can reasonably simulate the negative temperature phenomenon. The reason for this phenomenon is that the temperature rise reaction $C_7H_{16} + O_2 = C_7H_{15.2} + HO_2$ will generate HO_2 . The increase of HO_2 promotes the positive reaction $HO_2 + HO_2 = H_2O_2 + O_2$ and continuous temperature rise. The increase of temperature further promotes reactions $CH_3 + HO_2 = CH_3O + OH$ and $CH_3 + HO_2 = CH_4 + O_2$. The combustion process involves abundant free radical collision reactions, and the occurrence of these three elementary reactions causes a large consumption of HO_2 free radicals in the flame, which seriously reduces the overall combustion rate and inhibits the temperature rise. Subsequently, with the continuous chemical reaction in the flame, the flame temperature continues to rise, and the reaction $H_2O_2 (+M) = OH + OH (+M)$ starts in large quantities. The decomposition of H_2O_2 to generate OH is accompanied by much heat release, which promotes the rapid rise of flame temperature. The phenomenon of negative temperature coefficient is thus broken. With the temperature rise, the ignition delay time is shortened again.

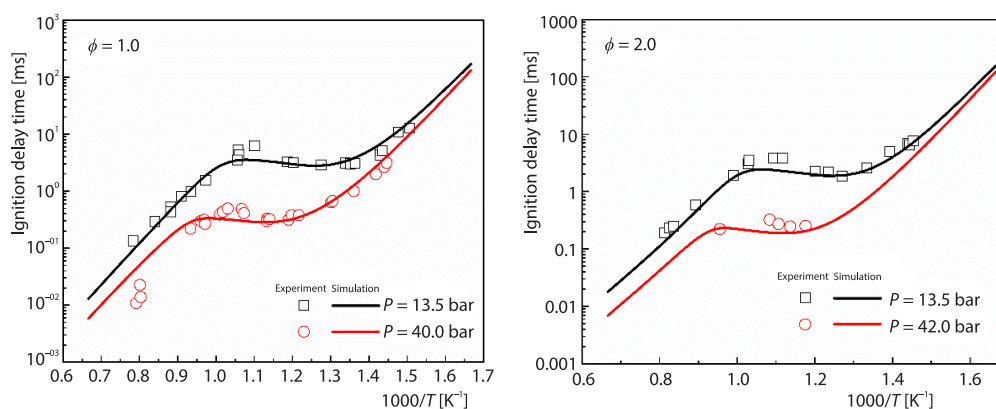


Figure 2. Measured (symbols) and predicted (lines) ignition delays of *n*-heptane

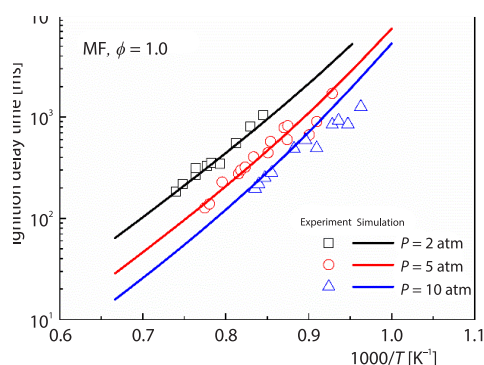


Figure 3. Measured (symbols) and predicted (lines) ignition delays of MF

component reaction in the combined mechanism is partially eliminated, resulting in a decrease of the low temperature reaction activity of MF and the prolonging of the ignition delay time.

Figure 3 compares the experimental [25] and simulated data of the ignition delay time of MF by the MF-diesel reduced mechanism. The temperature range is 900-1500 K, the equivalent ratio is 1, and the initial pressures are 2 atm, 5 atm and 10 atm. With the increase of pressure, the ignition delay time is shortened. Under the pressure of 2 atm and 5 atm, the ignition delay of MF simulation agrees well with the experimental data. At 10 atm pressure, the ignition delay of MF simulation is slightly larger than the experimental value at low temperature. This is because the MF reduced mechanism deletes a part of the low temperature reactions, and the small

Verification of laminar flame component concentration

In the verification of the combined mechanism, the ignition delay time is the most basic. To further ensure the reliability of the mechanism, we shall verify the laminar flame component concentration, which was calculated in a Chemkin-Pro flame simulator. The tem-

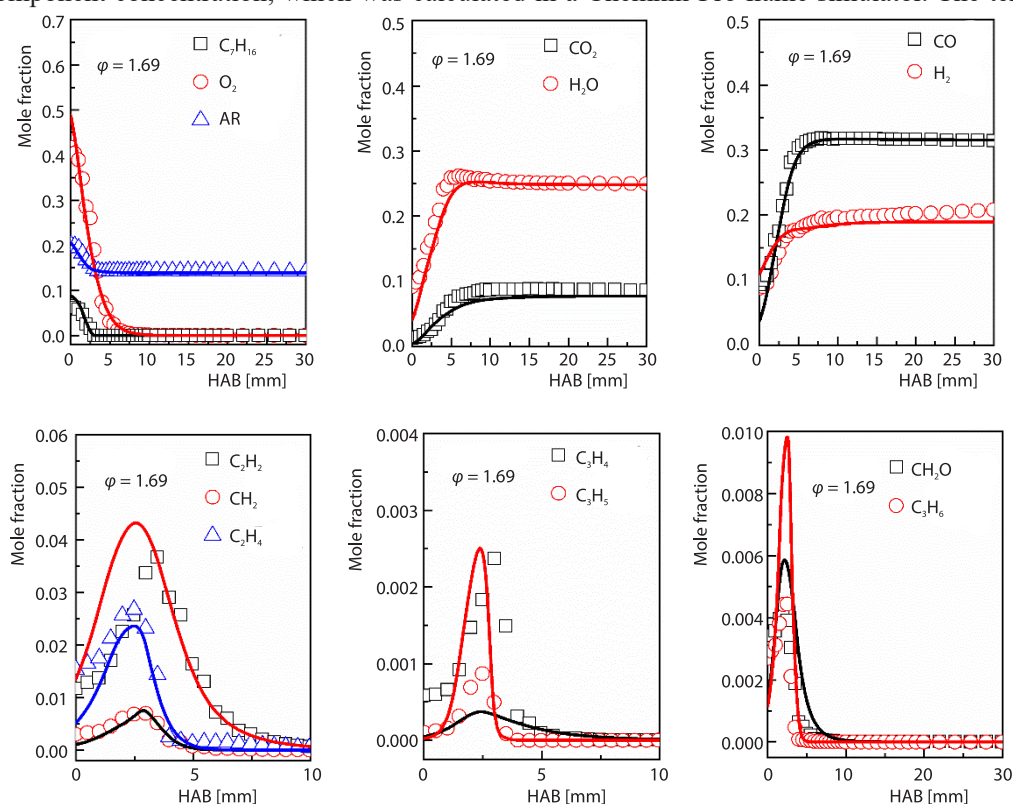


Figure 4. Measured (symbols) and predicted (lines) species profiles in premixed *n*-heptane flame

perature gradient of the actual experiment was used as the temperature setting in the simulation calculation. Figure 4 shows the verification of the molar concentration of the laminar flame species of *n*-heptane in the MF-diesel mechanism. The experimental data on the detailed species composition of *n*-heptane flame at 40 mbar in a premixed fuel-rich plate (equivalence ratio = 1.69) were obtained by Seidel *et al.* [26] through electron ionization molecular beam mass spectrometry (EI-MBMS). The simulation was carried out under the pressure of 0.04 bar, equivalence ratio of 1.69, temperature gradient of 380-2200 K, and initial flame velocity of 57.6 cm/s. The changing trends in the molar concentrations of H_2 , H_2O , CO , O_2 , AR , CO_2 and C_7H_{16} with the prolonging of flame distance do not significantly deviate from the experimental values. With the increase of HAB (height above burner), C_7H_{16} and O_2 consumption, the concentrations of H_2O , CO and CO_2 gradually increase. When HAB = 10 mm, it tends to be stable. The simulated data of some species (CH_2 , C_2H_2 , C_3H_4 , C_3H_6) are slightly different from the experimental data. The main reason is that to ensure its practicability in numerical simulation, the combined mechanism is adjusted by deleting the intermediate reactions and partial group reactions to only retain the skeleton reaction and partial C_2 - C_3 and H_2/O_2 reactions. In addition, the component concentration of the group is actually very low, and there will be some errors in the experimental measurement. These errors are within the acceptable range, but the overall fitting precision meets the requirements of practical application.

Figure 5 shows the simulated and experimental data of molar concentrations of the main components (H_2 , H_2O , CO , O_2 , AR , CO_2 , MF) in the MF premixed flame with equivalence

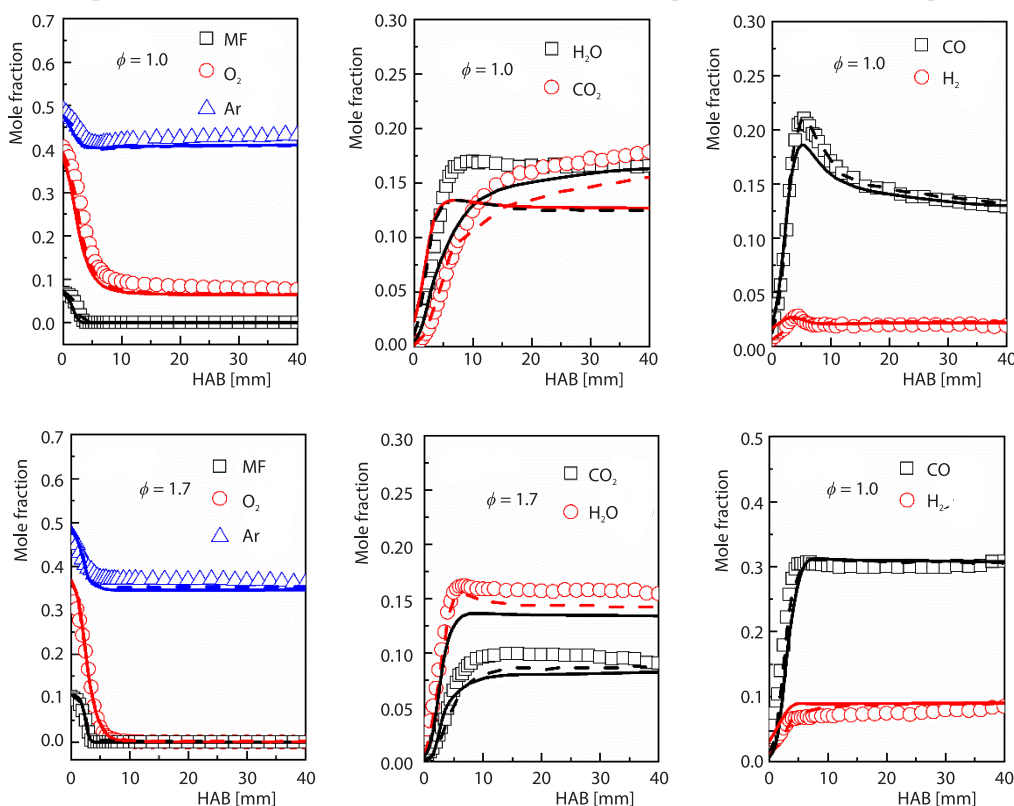


Figure 5. Measured (symbols) and predicted (lines) species profiles in premixed MF flames; solid lines: the present mechanism, dashed lines: the tran mechanism

ratio of 1 or 1.7. The experimental values were derived from EI-MBMS conducted by Tran *et al.* [12]. The simulation conditions were set according to the experimental conditions: pressure at 0.02 bar, temperature range of 400-2000 K, and initial flame velocity at 146 cm/s. Results show that the development trend of molar concentration distribution of each component with the increase of flame distance well agrees with the experimental data, but the concentrations of some products (CO_2 , H_2O , CO) are lower than the experimental data. This is because the MF-diesel reduced mechanism removes the unimportant reactions from the detailed MF mechanism, which may affect the predictive ability of those products.

Engine verification

The MF-diesel mechanism was verified by engine numerical simulation and reactivity controlled compression ignition (RCCI) test to ensure the accuracy of simulation calculation under engine related combustion conditions. Figure 6 shows the lay-out of the test bench. The RCCI test was conducted by a single cylinder engine with direct injection of diesel in the cylinder and MF injection in the inlet. The main technical parameters of the engine are shown in tab. 2. During the test, the speed of engine was kept at 1000 rpm. Diesel injection time was set at -12.5°CA aTDC (after top dead center), and the injection at pressure 60 MPa continued 5.4 millisecond. The constant calorific value method was adopted in the test, and the proportion of diesel fuel was the ratio of its calorific value injected into the cylinder to the total calorific value of the circulating fuel supply. The fuels used in the experiment were D100 and D55 that contained 100% and 55% diesel, respectively. Table 3 shows the physical properties of diesel and MF. The in-cylinder pressure and heat release rate curves under D100 and D55 conditions were compared with the simulation curves. To ensure the test conditions were consistent with the actual working environment of the engine, we set the water, oil and inlet temperatures at 85, 80 and 85 $^\circ\text{C}$, respectively, and the heating time at 30 min. The test was started after the inlet temperature sensor was stabilized. The diesel engine used in the experiment was a 9-hole nozzle injector. Only one-ninth of the combustion chamber model was adopted to improve the computational efficiency, fig. 7. The simulation setting was consistent with the tests. The calculation time was from -155°CA aTDC when the inlet valve was closed to 155°CA aTDC when the exhaust valve was opened. According to the experimental data, the simulated inlet pressure and temperature were 0.105 MPa and 333 K, respectively. The KH-RT crushing model, the Han and Reitz Wall heat transfer model, the SAGE combustion model, the O'Rourke collision model and the RNG $k-\varepsilon$ turbulence model were used in the calculations [27-32].

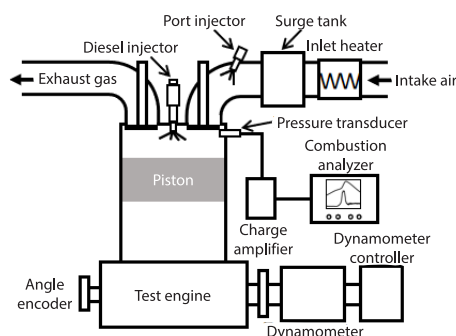


Figure 6. Test bench lay-out

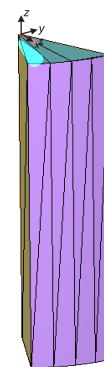


Figure 7. Combustion chamber model

Table 2. Engine specifications

Cylinder diameter	96 mm
Piston stroke	115 mm
Connecting rod length	210 mm
Valve number	4
Nozzle number	9
Nozzle diameter	0.15 mm
Spray cone angle	150°
Compression ratio	16.5

Table 3. Physical parameters of fuel

	Diesel	MF
Molecular formula	$C_{12}-C_{25}$	C_5H_6O
Derived cetane number	>50	8.9
Research octane number	—	131
Oxygen content [wt.%]	0	19.5
Density at 20 °C [kgm^{-3}]	820	913.2
Boiling point [K]	443-633	336
Viscosity at 40 °C [mm^2s^{-1}]	1.9-4.0	—
Low heating value [$MJkg^{-1}$]	42.5	30.4
Latent heating at 25 °C [$kJkg^{-1}$]	270-301	358
Auto-ignition temperature [°C]	246	450
Stoichiometric air-fuel ratio	14.3	10.05

Figure 8 compares in-cylinder pressure and heat release rate between the simulated and experimental data of D100 and D55 fuels in the engine. The simulation data of D55 are well consistent with the experimental data, and the ignition point and combustion phase are basically the same. However, the calculated peak cylinder pressure of D100 is lower than the experimental value. The reasons of such discrepancy may be attributed to the impact of turbulence on chemical kinetics was inaccurately considered in the predictions and only one lighter hydrocarbon fuels (*n*-heptane) were chosen as diesel surrogate fuel. In general, the fitting results of the simulation data and the experimental data are good, and this mechanism has certain accuracy in the application of engine numerical simulation.

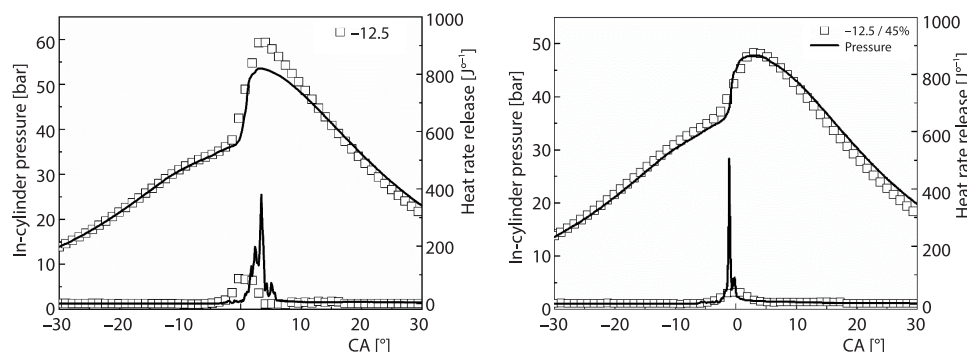


Figure 8. Experimental and simulated in-cylinder pressures and heat release rates for D100 and D55

Conclusions

A reduced MF-diesel mechanism containing 55 species and 190 reactions was constructed. Based on the detailed chemical reaction mechanism of MF studied by Tran *et al.* [12], the mechanism was simplified by the directed relation graph with error propagation, reaction path analysis, sensitivity analysis and rate of production analysis, and coupled into the diesel engine mechanism. Then the reaction rate constant A was optimized for the new MF-diesel simplified mechanism, and finally the MF-diesel reduced mechanism was obtained. Verifications of shock tube ignition delay, laminar flame species mole fraction distribution, and engine

cylinder pressure and heat release rate demonstrate the mechanism has excellent stability and accuracy and is applicable for numerical simulation research under engine-related combustion conditions.

References

- [1] Kalong, M., *et al.*, Hydrogen-Free Hydrogenation of Furfural to Furfuryl Alcohol and 2-Methylfuran over Ni and Co-Promoted Cu/ γ -Al₂O₃ Catalysts, *Fuel Processing Technology*, 214 (2021), 106721
- [2] Pepiot-Desjardins, P., *et al.*, Structural Group Analysis for Soot Reduction Tendency of Oxygenated Fuels, *Combustion and Flame*, 154 (2008), 1-2, pp. 191-205
- [3] Yanowitz, J., *et al.*, Utilization of Renewable Oxygenates as Gasoline Blending Components, Contract, Technical Report, NREL/TP-5400-50791, 2011
- [4] Wei, H., *et al.*, Experimental Investigation on the Combustion and Emissions Characteristics of 2-Methylfuran Gasoline Blend Fuel in Spark-Ignition Engine, *Applied Energy*, 132 (2014), Nov., pp. 317-324
- [5] Hoang, A. T., The 2-Methylfuran (MF) as a Potential Biofuel: A thorough Review on the Production Pathway from Biomass, Combustion Progress, and Application in Engines, *Renewable and Sustainable Energy Reviews*, 148 (2021), 111265
- [6] Wang, C., *et al.*, Combustion Characteristics and Emissions of 2-Methylfuran Compared to 2,5-Dimethylfuran, Gasoline and Ethanol in a DISI Engine, *Fuel*, 103 (2013), Jan. pp. 200-211
- [7] Katinska, A., Comprehensive Review of the Impact of 2,5-Dimethylfuran and 2-Methylfuran on Soot Emissions: Experiments in Diesel Engines and at Laboratory-Scale, *Energy and Fuels*, 34 (2020), 6, pp. 6598-6623
- [8] Xiao, H. L., *et al.*, Effects of Pilot Injection on Combustion and Emissions Characteristics Using 2-Methylfuran/Diesel Blends in a Diesel Engine, *Thermal Science*, 24 (2020), 1A, pp. 1-11
- [9] Liu, H. Y., *et al.*, Combustion Characteristics and Engine Performance of 2-Methylfuran Compared to Gasoline and Ethanol in a Direct Injection Spark Ignition Engine, *Fuel*, 299 (2021), 120825
- [10] Sirjean, B., *et al.*, Shock Tube and Chemical Kinetic Modelling Study of the Oxidation of 2,5-Dimethylfuran, *Journal of Physical Chemistry A*, 117 (2013), 7, pp. 1371-1392
- [11] Lifshitz, A., *et al.*, Thermal Decomposition of 2,5-Dimethylfuran. Experimental Results and Computer Modelling, *Journal of Physical Chemistry A*, 102 (2011), 52, pp. 10655-10670
- [12] Tran, L. S., *et al.*, Combustion Chemistry and Flame Structure of Furan Group Biofuels Using Molecular-Beam Mass Spectrometry and Gas Chromatography – Part II: 2-Methylfuran, *Combustion and Flame*, 161 (2014), 3, pp. 766-779
- [13] Liu, D., Combustion Chemistry and Flame Structure of Furan Group Biofuels Using Molecular-Beam Mass Spectrometry and Gas Chromatography – Part I: Furan, *Combustion and Flame*, 161 (2014), 3, pp. 748-765
- [14] Casimir, Togbe, *et al.*, Combustion Chemistry and Flame Structure of Furan Group Biofuels Using Molecular-Beam Mass Spectrometry and Gas Chromatography – Part III: 2,5-Dimethylfuran, *Combustion and Flame*, 161 (2014), 3, pp. 780-797
- [15] Tian, Z., *et al.*, An Experimental and Kinetic Investigation of Premixed Furan/Oxygen/Argon Flames, *Combustion and Flame*, 158 (2011), 4, pp. 756-773
- [16] Tay, K. L., *et al.*, Development of a Highly Compact and Robust Chemical Reaction Mechanism for Unsaturated Furan Oxidation in Internal Combustion Engines Via a Multiobjective Genetic Algorithm and Generalized Polynomial Chaos, *Energy and Fuels*, 34 (2020), 1, pp. 936-948
- [17] Chang, Y., *et al.*, Development of a Skeletal Mechanism for Diesel Surrogate Fuel by Using a Decoupling Methodology, *Combustion and Flame*, 162 (2015), 10, pp. 3785-3802
- [18] Somers, K. P., *et al.*, A High Temperature and Atmospheric Pressure Experimental and Detailed Chemical Kinetic Modelling Study of 2-Methyl Furan Oxidation, *Proceedings of the Combustion Institute*, 34 (2013), 1, pp. 225-232
- [19] Somers, K. P., *et al.*, A Comprehensive Experimental and Detailed Chemical Kinetic Modelling Study of 2,5-Dimethylfuran Pyrolysis and Oxidation, *Combustion and Flame*, 160 (2013), 11, pp. 2291-2318
- [20] Somers, K. P., *et al.*, The Pyrolysis of 2-Methylfuran: A Quantum Chemical, Statistical Rate Theory and Kinetic Modelling Study, *Physical Chemistry Chemical Physics*, 16 (2014), 11, pp. 5349-5367
- [21] Wang, H., *et al.*, A Reduced Toluene Reference Fuel Chemical Kinetic Mechanism for Combustion and Polycyclic-Aromatic Hydrocarbon Predictions, *Combustion and Flame*, 162 (2015), 6, pp. 2390-2404
- [22] Li, S., *et al.*, Development of a Phenomenological Soot Model Integrated with a Reduced TRF-PAH Mechanism for Diesel Engine Application, *Fuel*, 283 (2021), 118810

- [23] Ciezki, H. K., Adomeit, G., Shock-Tube Investigation of Self-Ignition of n-Heptane-Air Mixtures under Engine Relevant Conditions, *Combustion and Flame*, 93 (1993), 4, pp. 421-433
- [24] Hartmann, M., *et al.*, Auto-Ignition of Toluene-Doped n-Heptane and Iso-Octane/Air Mixtures: High-Pressure Shock-Tube Experiments and Kinetics Modelling, *Combustion and Flame*, 158 (2011), 11, pp. 72-178
- [25] Eldeeb, M.A., Akih-Kumgeh, B., Reactivity Trends in Furan and Alkyl Furan Combustion, *Energy and Fuels*, 28 (2014), 10, pp. 6618-6626
- [26] Seidel, L., *et al.*, Comprehensive Kinetic Modelling and Experimental Study of a Fuel-Rich, Premixed n-Heptane Flame, *Combustion and Flame*, 162 (2015), 5, pp. 2045-2058
- [27] Han, Z. Y., Reitz R. D., Turbulence Modelling of Internal Combustion Engines Using RNG $k-\epsilon$, Models, *Combustion Science and Technology*, 106 (1995), 4-6, pp. 267-295
- [28] Babajimopoulos, A., *et al.*, A Fully Coupled Computational Fluid Dynamics and Multi-Zone Model with Detailed Chemical Kinetics for the Simulation of Premixed Charge Compression Ignition Engines, *International Journal of Engine Research*, 6 (2005), 5, pp. 497-512
- [29] Amsden, A. A., *et al.*, The KIVA-2: A Computer Program for Chemically Reactive Flows with Sprays, NASA Sti/Recon Technical Report N, NASA, Washington DC, 1989
- [30] Reitz, R. D., Diwakar, R., *Structure of High-Pressure Fuel Sprays*, SAE Technical Paper, 870598
- [31] Reitz, R. D., Diwakar, R., *Effect of Drop Breakup on Fuel Sprays*, SAE Technical Paper, 860469
- [32] Han, Z.Y., Reitz, R. D., A Temperature Wall Function Formulation for Variable-Density Turbulent Flows with Application Engine Convective Heat Transfer Modelling, *International Journal of Heat and Mass Transfer*, 40 (1997), 3, pp. 613-625