

Modeling of Auto-Ignition and Combustion Processes for Dual-Component Fuel Spray

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ABSTRACT

Auto-ignition and combustion processes of dual-component fuel spray were numerically studied. A source code of SUPERTRAPP (developed by NIST), which is capable of predicting thermodynamic and transportation properties of pure fluids and fluid mixtures containing up to 20 components, was incorporated into KIVA3V to provide physical fuel properties and vapor-liquid equilibrium calculations. Low temperature oxidation reaction, which is of importance in ignition process of hydrocarbon fuels, as well as negative temperature coefficient behavior was taken into account using the multistep kinetics ignition prediction based on Shell model, while a global single-step mechanism was employed to account for high temperature oxidation reaction.

Computational results with the present multi-component fuel model were validated by comparing with experimental data of spray combustion obtained in a constant volume vessel. The results showed a good agreement in terms of spray tip penetration, liquid length, ignition delay and so on, for several kinds of dual-component fuels. Additional investigation into a combustion control methodology using dual-component fuel, which aims to mitigate combustion rate of premixed charge, was performed. Consequently, the feasibility of this approach was confirmed.

INTRODUCTION

Currently, growing interest in global warming and energy crisis has promoted production of alternative fuels for internal combustion engines. Some of alternative fuels have physical and chemical properties different from conventional ones. For example, reactivity and volatility of gas to liquid (GTL) and dimethyl ether (DME) are higher than those of diesel fuel, and inversely those of light cycle oil (LCO) are lower. The fuel properties of the next-generation energy sources can have a significant impact on mixture preparation, and hence ignition and combustion characteristics, while the operation with them would be a possible approach to achieve low emissions engine system because a wide variety of them increases a flexibility of mixture preparation and ignition controllability.

Since such alternative fuels are generally used as a mixture with conventional fuels, due to the limitation in terms of amount of production, numerous studies have addressed fuel effects in internal combustion engines [1, 2, 3]. In addition, there are other researches aiming to actively use the mixing effects of alternative fuels [4, 5, 6]. However, although they demonstrated that the combustion and emissions were drastically improved by optimizing transportation properties and volatility as well as chemical reaction process, further analyses at fundamental level would be required to generalize the knowledge and to estimate the effective utilization methodology.

The authors have performed a basic research to demonstrate a potential benefit of binary fuels consisting of different reactivity and volatility components for over a decade [7, 8, 9]. According to the experimental and numerical investigations, it has been clear that the interaction between the molecules affect vapor-liquid equilibrium characteristics during droplet vaporization process. Specifically, mixing different volatility components forms two-phase region where liquid and vapor of both components co-exist so that alter the volatility of both components, as schematically shown in pressure-temperature diagram of Fig.1. In addition, after fuel injection, droplets passing across the bubble point curve form a mixture in which the vapor of the high volatility component is dominant. Since the two-phase region gradually shifts to lower pressure and higher pressure side due to the decrease of the high volatility component in the droplet, this phenomenon, so-called batch-distillation, leads to spatial stratification of two vapor components in a fuel spray [9, 10], as shown in Fig.2. Such stratified two components would yield thermal stratification prior to the onset of high temperature oxidation reaction (HTR) if they had different low temperature oxidation chemistry each other. The thermal stratification would discretize the appearance of HTR spatially and temporally, and hence the combustion process could be controlled by adjusting the distribution location of the two components and by selecting the combinations of the components.

To demonstrate a potential of this approach, a multi-dimensional simulation model for multi-component fuel has been developed [11]. This model implements the predictions of transportation properties and liquid-vapor equilibrium of dual-component fuel by using SUPERTRAPP of NIST [12] with taking into account the effects of high-pressure as well as real gas effect.

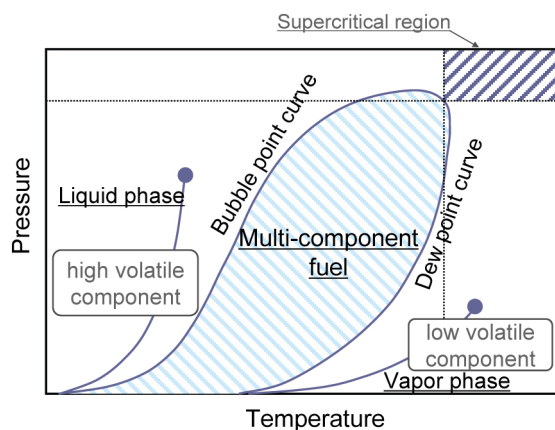


Fig.1. Schematic of pressure-temperature diagram of pure fuels and multi-component fuel

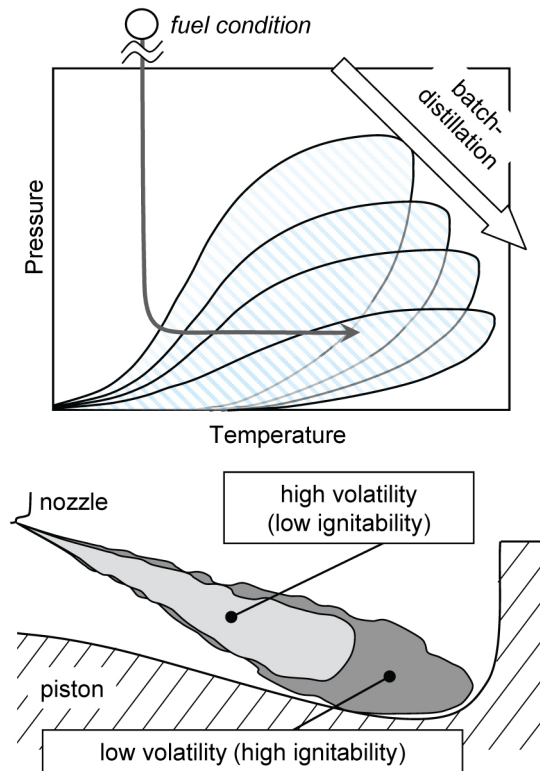


Fig.2. Schematic of vaporization process of multicomponent-fuel and batch-distillation phenomenon

The present study expanded this multi-component fuel spray model to ignition and combustion simulation as well as minor changes of sub-models. The model adapted a multistep kinetics ignition prediction based on Shell model [13] into the multi-component fuel spray model to express low temperature oxidation reaction of hydrocarbon fuels. High temperature oxidation reaction was expressed by a combination of global single step mechanism and the eddy-dispersion model of Magnussen et al. [14].

Studies have been made to validate the present model and additionally to gain insight into the physics and chemical process involved in spray-combustion of dual-component fuels by comparing numerical results with experimental ones, including spray characteristics, heat release rate and combustion location obtained in a constant volume vessel. Furthermore, the feasibility of the approach shown in Fig.2 was investigated applying the present model to engine simulation.

MODEL FORMULATION

The KIVA3V code [15] was used in this study with improvements of the spray and ignition models. The flowchart of the present model is shown in Fig.3. More details on the multi-component vaporization model have

already been reported in the literature [11] and hence essential points of sub-models are discussed here.

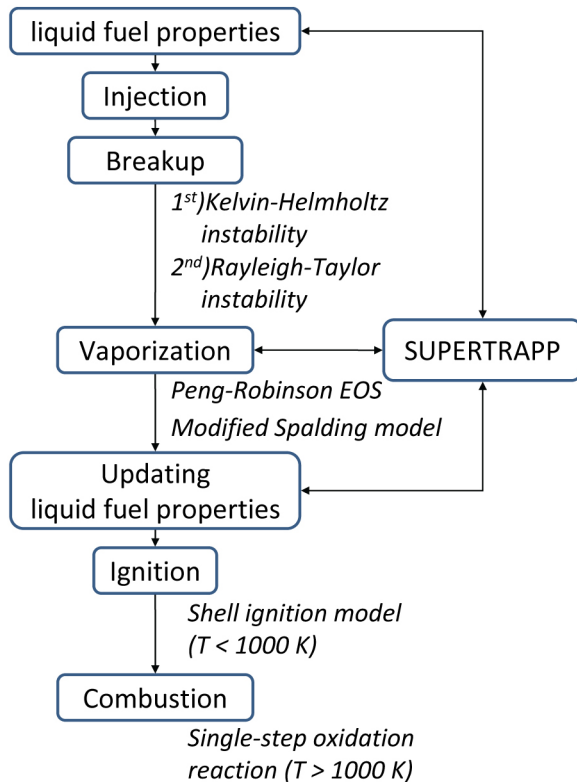


Fig.3. Flowchart of the present model

DROPLET BREAKUP MODEL

In order to solve droplet breakup, the original multi-component fuel spray model had employed the Taylor Analogy Breakup (TAB) model with an optimization of model constants [11]. On the other hand, the Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) model [16] was incorporated to accurately predict liquid phase penetration. Although this model have several model constants, once a combination of the model constants were found to give a good agreement with experimental liquid phase penetration of a single component fuel, the present study adapted the constants for all fuels.

DROPLET VAPORIZATION

Early studies on multi-component fuel vaporization have developed several models. In the recent past it has become more popular to model multi-component fuel by means of continuous thermodynamics with a continuous distribution function that specifies the mole fraction in terms of the molecular weight [17]. However, this approach is difficult to represent the effects of interaction between the molecules and hence the histories of two-phase region. Jin and Borman proposed a model that accounts for high-pressure and non-ideal gas effects in multi-component fuel vaporization using

Redlich-Kwong equation of state [18]. This model was applied to three-dimensional simulation of diesel spray and combustion with the discrete representation of the multi-component mixture [19]. In addition, Ra and Reitz also used the discrete multi-component approach using a combination of Raoult's law and Clausius-Clapeyron equation [20]. Applying this approach to multi-component fuels which have wide range boiling point components, the batch-distillation phenomenon was predicted.

The authors also have developed a multi-component fuel vaporization model [11]. To evaluate the effects of interaction between molecules, high-pressure and non-ideal gas, a source code of SUPERTRAPP developed in NIST was incorporated into KIVA3V. This code calculates vapor-liquid equilibrium and gives phase compositions with Peng-Robinson equation of state [12]. Hence it is possible to handle discrete multi-component vaporization process with solving the phase equilibrium relationship for all the components in both phases. In addition, the solubility of gas in the droplet was taken into account, while omitting internal circulation of the liquid and temperature gradient within droplets.

Due to the batch-distillation, the mixture fraction within droplets would be changed as time goes by. All the fuel properties of droplet parcels were updated in every numerical timestep with taking into account both the temperature and pressure effects as well as mixing fraction. The SUPERTRAPP code calculates thermodynamic and transport properties based on extended corresponding states, in which the correlations for the propane reference fluid are used. Representation of mixtures is based on the one-fluid corresponding-states principle. The mixture is first characterized as a hypothetical pure fluid and then the resulting hypothetical pure fluid is related to the reference fluid. Mixing rules are adapted with taking into account the binary interaction parameters obtained from the generalized method of Nishiumi et al. [21]. The more details on the prediction are summarized in the literature [22].

IGNITION MODEL

The oxidation reaction lower than 1000 K was predicted according to the multistep kinetics Shell ignition model developed by Halstead et al. [13]. It includes eight reaction steps between five generalized species, specified as:





where RH indicates the fuel, R^* is the generalized radical, Q is an unstable intermediate agent, B is the branching agent, and P denotes oxidized products such as CO, CO₂ and H₂O. The rate terms f_i are expressed as follows:

$$f_i = A_{f_i} \cdot \exp\left(\frac{-E_{f_i}}{R \cdot T}\right) \cdot [O_2]^{x_i} \cdot [RH]^{y_i} \quad (1)$$

where R is universal gas constant and T is surrounding gas temperature. The kinetic parameters, k_p , k_b and k_t , are expressed in the Arrhenius form as:

$$k_i = A_i \cdot \exp\left(\frac{-E_{f_i}}{R \cdot T}\right) \quad (2)$$

k_p is given by the following expression with three rate coefficients:

$$k_p = \left[\frac{1}{k_{p_1} \cdot [O_2]} + \frac{1}{k_{p_2}} + \frac{1}{k_{p_3} \cdot [RH]} \right]^{-1} \quad (3)$$

The species concentrations are solved by numerically integrating the differential equations. The heat release due to the reaction can be expressed by the [reaction \(R2\)](#). For the implementation of multi-dimensional simulation, the Shell model was modified to maintain the mass conservation according to the procedure of Sch  pert  ns and Lee [\[23\]](#).

In the ignition and combustion simulation of multi-component fuel spray, the mixture compositions are different in every computational cell since each component could be vaporizing at different rate each other due to their volatility differentials. Thus, the reaction rate should be separately given in each cell. According to the sensitivity analysis of

Kong and Reitz [\[24\]](#), the formation of intermediate agent Q is thought to be the crucial reaction leading to high temperature oxidation reaction. There are several studies that report the successful representation of ignition processes by changing rate parameters of the [reaction \(R4\)](#) [\[25, 26\]](#). In particular, with respect to multi-component fuels, the activation energy E_{f4} was given as a function of the cetane number calculated by mixture compositions [\[17, 27\]](#). Various correlations relating cetane number and mixture compositions have been proposed [\[28\]](#). For example, Rose and Cooper [\[29\]](#) have approximated the relation between cetane number ($CN_{paraffins}$) and mean molecular weight (θ) of the fuel vapor as following:

$$CN_{paraffins} = -4.2438 \cdot 10^{-6} \theta^3 + 1.7080 \cdot 10^{-3} \theta^2 + 0.14675\theta + 29.295 \quad (4)$$

Furthermore, [Eq.\(4\)](#) has been modified by the correlation given by Glavinovski et al. [\[30\]](#):

$$CN = 30 + 0.221182 \cdot (CN_{paraffins} - 47.18) \quad (5)$$

However, their available ranges are limited in diesel-like fuels. In fact, the results applying such correlations to fuels of interest in this study showed considerable disagreement between the prediction and the experiment (see [Fig.8](#)).

Overall, the present study solved the above rate equations individually against mixture compositions. In addition, the generalized species produced by each fuel were specified as R^*_i , Q_i and B_i , where i denotes a kind of fuel, because sharing the generalized species R^* , Q and B among the mixture compositions led to prompt ignition. That is, this approach assumes that there is no chemical interaction between components, and hence the use would be restricted to normal paraffin and/or iso-paraffin which have no strong inhibitor effect on low temperature oxidation reaction [\[31\]](#). Further improvement may be accomplished with taking into account the interference among the generalized species. The activation energy of fuel i , $E_{f4,i}$ was given by the following expression with cetane number (CN) as:

$$E_{f4,i}^* = E_{f4} \frac{a}{CN + b} \quad (6)$$

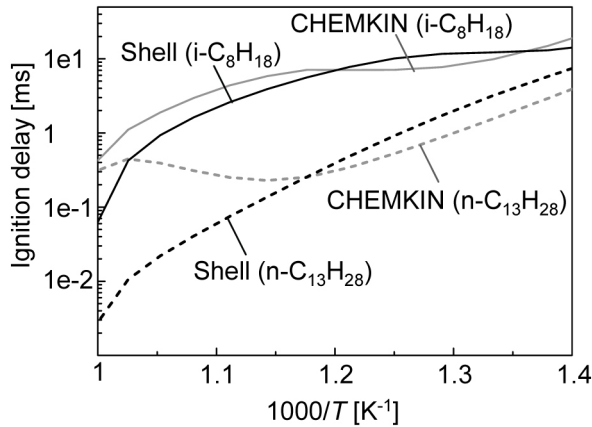


Fig.4. Comparison of ignition delay of $n\text{-C}_{13}\text{H}_{28}$ and $i\text{-C}_8\text{H}_{18}$ between Shell model and CHEMKIN ($p_a=3.6$ MPa, $\Phi=1.0$)

where a and b are constants determined to fit the results using the detailed chemical kinetic calculation of CHEMKIN. Figure 4 shows a comparison of ignition delay between the Shell model and CHEMKIN at constant volume. The calculation was implemented at an equivalence ratio of 0.5 and pressure of 3.6 MPa for a sweep of initial temperature. To determine the ignition delay of n -tridecane ($n\text{-C}_{13}\text{H}_{28}$, $CN=88$) and i -octane ($i\text{-C}_8\text{H}_{18}$, $CN=12$), detailed mechanisms of Lawrence Livermore National Laboratory [32, 33] were employed in the CHEMKIN calculation, while the Shell model used the constants of PRF90 model proposed by Theobald and Cheng [25] except for A_{f4} (set at $7.0e5$) and $E_{f4,i}$. The Shell predictions qualitatively reflect the difference of ignition delays in both the fuels, although mismatching at high initial temperature conditions.

COMBUSTION MODEL

A simplified single step oxidation model pre-installed into KIVA3V was used to predict oxidation reactions higher than 1000 K. Based on the local compositions of the fuel, the multi-component species were assumed to be a mole-averaged fuel.

The eddy-dispersion model developed by Magnussen et al. [14] was used to consider the turbulent mixing-controlled combustion.

NUMERICAL CONDITION

The predicted results were compared with the experimental ones previously reported by the authors [34], in order to the accuracy of the present model and to gain insight into physics and chemical processes of dual component fuels.

The experiments were conducted in a constant volume vessel which had a pan-cake type combustion chamber with 70 mm in diameter and 26 mm in width. The procedure is similar to Kamimoto et al. [35] and Siebers [36]. The premixed, combustible-mixture composed of ethylene, oxygen and nitrogen was spark-ignited to get the ambient with high temperature and high pressure. The mixture consisted of excess oxygen molecule so that 21 mol.% oxygen was remained in the gas after the spark-ignition. In addition, to investigate the spray characteristics without ignition, the inert ambient without oxygen molecule was prepared by changing the premixed gas composition. After the hot gases decreased the temperature due to heat transfer to the wall, the fuel was injected into the environment. The in-cylinder pressure analysis and shadowgraph and chemiluminescence imaging offer the ignition and combustion processes.

Several kinds of pure fuels summarized in Table 1 were tested in this study. N -tridecane ($n\text{-C}_{13}\text{H}_{28}$) which has high reactivity and high boiling point was used as a diesel-like fuel. The other fuels have low reactivity, while the boiling points are different each other. By mixing them into $n\text{-C}_{13}\text{H}_{28}$, the effects of the fuel volatility were evaluated. Figure 5 shows the pressure-temperature diagram of the dual-component fuels calculated by SUPERTRAPP.

In the experiment, heptamethylnonane ($i\text{-C}_{16}\text{H}_{34}$) was tested as a low reactivity and low volatility fuel. However, since the libraries of SUPERTRAPP and KIVA3V have no data relating to $i\text{-C}_{16}\text{H}_{34}$, hexadecane ($n\text{-C}_{16}\text{H}_{34}$) which has volatility similar to $i\text{-C}_{16}\text{H}_{34}$ was simulated as a substitute, assuming that it has low reactivity.

Table 1. Properties of fuels tested

Fuel	Boiling point [K]	Density [kg/m ³]	Cetane No. [-]	Octane No. [-]
i -pentane ($i\text{-C}_5\text{H}_{12}$)	301	615	-	92
i -octane ($i\text{-C}_8\text{H}_{18}$)	372	688	12	100
n -tridecane ($n\text{-C}_{13}\text{H}_{28}$)	510	756	88	-
n -hexadecane ($n\text{-C}_{16}\text{H}_{34}$)	560	770	100	-
heptamethyl nonane ($i\text{-C}_{16}\text{H}_{34}$)	520	793	15	-