ENGINE FUELS TYPICALLY CONSIST OF MANY DIFFERENT HYDROCARBON COMPONENTS THAT VAPORIZE AT DIFFERENT BOILING POINT TEMPERATURES. IN ORDER TO KEEP COMPUTATIONAL COSTS LOW, HOWEVER, TRADITIONAL ENGINE COMPUTATIONS WERE MADE WITH THE ASSUMPTION OF A SINGLE COMPONENT FUEL WITH A SINGLE BOILING POINT. UNDER THIS ASSUMPTION, THE FASTER VAPORIZATION OF LIGHTER COMPONENTS AND THE SLOWER VAPORIZATION OF HEAVIER COMPONENTS ARE NOT CAPTURED. CONSEQUENTLY, THE MIXING AND COMBUSTION PROCESS CAN NOT BE ADEQUATELY REPRESENTED. THEREFORE, COMPUTATIONS WITH MULTICOMPONENT FUEL CAPABLE OF REPRESENTING THIS EFFECT ARE DESIRED.

AN ESSENTIAL PROBLEM FOR MULTICOMPONENT FUEL COMPUTATIONS IS HOW TO Describe FUEL VAPORIZATION. DIFFERENT FROM SINGLE-COMPONENT SUBSTANCE, MULTICOMPONENT FUELS VAPORIZE IN A MORE TRANSIENT MANNER. IN GENERAL, THE COMPOSITION ALWAYS VARIES, AND ITS SPATIAL DISTRIBUTION IS ALSO NON-UNIFORM. THERE WERE INTENSIVE STUDIES IN LITERATURES AND SEVERAL KINDS OF MODELS HAVE BEEN DEVELOPED TO DESCRIBE THIS UNSTEADY VAPORIZATION BEHAVIOR FOR MULTICOMPONENT DROPLET AND FILM (TWO FORMS THAT FUEL EXISTS IN ENGINES). HOWEVER, MOST OF THESE MODELS ARE EITHER COMPUTATIONALLY INTENSIVE OR INSUFFICIENTLY ACCURATE.

THIS PAPER OUTLINED A NUMERICAL METHOD FOR MULTICOMPONENT FUEL COMPUTATIONS WITH RELATIVELY LOW COMPUTATIONAL COST WHILE WITH HIGH ACCURACY. THE STARTING POINT IS THE KIVA-3V CODE [1], WHICH HAS BEEN EXTENSIVELY USED IN ENGINE COMPUTATIONS DUE TO ITS CAPACITY IN MODELING TURBULENCE, SPRAY DYNAMICS AND CHEMICAL REACTION AND ITS FLEXIBILITY IN HANDLING THE ENGINE-LIKE GEOMETRY. HOWEVER, THIS CODE IS LIMITED TO SINGLE COMPONENT FUELS. EXTENDED EFFORTS HAVE BEEN MADE TO MODEL MULTICOMPONENT FUEL EFFECTS [2-6]. IN THIS STUDY, THE SINGLE COMPONENT REPRESENTATION FOR FUEL WAS EXTENDED TO A MULTICOMPONENT REPRESENTATION, AND PART OF PROPERTY EVALUATION METHODS WERE REPLACED BY MORE ACCURATE METHODS. TWO NEWLY DEVELOPED MULTICOMPONENT VAPORIZATION MODELS FOR DROPLET AND FILM WERE USED TO DESCRIBE FUEL VAPORIZATION IN ENGINES [4-6]. THESE TWO MODELS TAKE INTO ACCOUNT IMPORTANT MECHANISMS INVOLVED, SUCH AS PREFERENTIAL VAPORIZATION, FINITE DIFFUSION, INTERNAL CIRCULATION, SURFACE REGRESSION, AND NON-IDEAL BEHAVIOR IN HIGH-PRESSURE ENVIRONMENTS [4-6]. HOWEVER, THEIR COMPUTATIONAL COST IS ONLY SLIGHTLY HIGHER THAN THOSE OF THE VAPORIZATION MODELS IN THE ORIGINAL CODE AND IS MUCH LOWER THAN THOSE OF OTHER MODELS WITH SIMILAR ACCURACY IN LITERATURES [4-6].

THE DEVELOPED METHOD WAS USED TO INVESTIGATE AIR/FUEL MIXTURE PREPARATION IN A PORT FUEL INJECTION (PFI) SPARK IGNITION ENGINE UNDER THE COLD STARTING CONDITION SINCE MULTICOMPONENT FUEL EFFECTS ARE MOST SIGNIFICANT UNDER THIS CONDITION. THE COMPUTED ENGINE IS A FOUR-VALVE PENT-ROOF ENGINE. THE FUEL IS COMPOSED OF FOUR COMPONENTS AND IT PRODUCES A DISTILLATION CURVE SIMILAR TO THAT OF AN ACTUAL GASOLINE FUEL [7]. COMPUTATIONAL RESULTS WERE COMPARED WITH EXPERIMENTAL RESULTS OF EXCIPLEX FLUORESCENCE MEASUREMENTS FOR FUEL VAPOR IN-CYLINDER DISTRIBUTION. THE TIME-RESOLVED INFORMATION ON LIQUID AND VAPOR MASS WAS PROVIDED AND DISCUSSED. EFFECTS OF ENGINE OPERATING PARAMETERS INCLUDING SWIRL INTENSITY, ENGINE SPEED AND INJECTION TIMING ON THE IN-CYLINDER FUEL DISTRIBUTION WERE ALSO PRESENTED.

NUMERICAL MODEL

IN THE KIVA-3V CODE, PARCEL REPRESENTATION IS USED FOR LIQUID FUEL. EACH PARCEL (DROPLET OR FILM) IS TRACKED INDIVIDUALLY, AND THE TWO-WAY COUPLING BETWEEN THE LIQUID FUEL AND THE CARRYING GAS IS IMPLEMENTED BY A POINT-SOURCE-VOLUME METHOD [1]. TWO MAJOR ISSUES NEEDED ADDRESS ARE HOW TO DETERMINE THE MOMENTUM, MASS AND HEAT TRANSFER RATES BETWEEN TWO PHASES AND HOW TO DESCRIBE THE RESPONSES OF THE PARCEL, AND THESE ISSUES ARE COVERED BY THE TWO VAPORIZATION MODELS PRESENTED BELOW.

DROPLET VAPORIZATION MODEL


$$\omega_i = \frac{D_{gi} \cdot Sh_i \cdot \zeta_i \cdot B_i}{d}$$  \hspace{1cm} (1)
where \( \omega \) is the vaporization rate, \( D_g \) the gas phase mass diffusivity coefficient, \( Sh \) the Sherwood number, \( \zeta \) the correction factor for the effect of Stephan flow, \( B \) the transfer number, and \( d \) the droplet diameter. Subscript ‘i’ stands for component \( i \).

Due to the diffusion resistance inside the droplet and preferential vaporization, the property distributions within the droplet are non-uniform in general. In this study, this non-uniformity represented by the difference between the surface and average values is given by an ordinary differential equation with respect to time \( t \) [5],

\[
\frac{d \Phi_d}{dt} = \frac{0.2E(P_{ev})\phi R/D_i - \Phi_d}{E(P_{ev})R^2/4.49^2 D_i}
\]

where \( \Phi_d \) is the difference between the surface and average values for the temperature \( T \) or mass fraction \( Y_i \), \( D_i \) the effective thermal or mass diffusivity coefficient, \( \phi \) the heat or species mass diffusional flux at the droplet surface, \( R \) the droplet radius, and \( E \) the correction factor for the effect of surface regression.

The effect of surface regression is quantified by a non-dimensional variable \( P_{ev} \) defined as [5]

\[
P_{ev} = R \sum \omega_i / D_i
\]

which represents the ratio of the thermal or mass diffusional time scale to the surface regression time scale. When \( P_{ev} \) is small (i.e., slow vaporization rate), the effect of surface regression is negligible and thus the steady profiles of temperature and mass fractions within the droplet are quadratic. However, this quadratic profile will shift to a distribution showing a structure similar to that of the boundary layer flow, with decreasing boundary layer thickness as \( P_{ev} \) increases [5]. \( E(P_{ev}) \) is defined as the ratio of the difference of surface and average values to the difference at \( P_{ev} = 0 \) subject to the same boundary conditions. Through theoretical analysis, the authors found the expression for \( E(P_{ev}) \) [5], and it is given by,

\[
E(P_{ev}) = \left[ \frac{8 \int_0^r \frac{\delta \Phi}{\delta r} dr - 3 \frac{\delta}{\delta r} \left( \int_0^r \left( \frac{\delta \Phi}{\delta r} \right) r^2 dr \right) }{ \int_0^r \left( \frac{\delta \Phi}{\delta r} \right) r^2 dr } \right]_{P_{ev}=0}
\]

**Film Vaporization Model**

Based on the boundary layer equations and the Prandtl mixing-length theory, O’Rourke and Amsden [9] developed a modified wall function to determine the transfer rate between the film and the adjacent gas. Following the same strategy, the authors extended it to include multicomponent fuel effects, and the species vaporization rate \( \omega_i \) is given by [6]

\[
\omega_i = H_{Y_i} \zeta, \quad (5)
\]

where \( H_{Y_i} \) is the overall diffusivity, \( \zeta \) the correction factor for the effect of Stephan flow, and \( B \) the transfer number. Subscript ‘i’ refers to component \( i \).

The mass fraction and temperature distributions within the film are non-uniform as well because of finite thermal and mass diffusion speeds. The authors recently developed a model for this non-uniformity using a third-order polynomial to simulate the temperature and mass fraction unsteady profiles within the film. This model reduces the governing equations for mass and energy transport to a set of ordinary differential equations \[29\]. With this model, the surface temperature is given by [6]

\[
\frac{dT_s}{dt} = \frac{\alpha_i}{k_i} \left( \frac{q \delta}{\delta^2} - 3 T_s - T_w + 4 T_m \right)
\]

where \( T_s \) is the film surface temperature, \( \alpha_i \) is the liquid phase thermal diffusivity coefficient, \( \delta \) is the film thickness, \( q \) the heat flux to the film, \( k_i \) the liquid phase conductivity coefficient, \( T_w \) the wall temperature, and \( T_m \) the film average temperature. The difference between the surface and average mass fractions for component \( i \) is given by [6]

\[
\frac{d(Y_{(s_i)} - Y_{(mi)})}{dt} = \frac{4 \Gamma_{(s_i)}^i}{\rho \delta^2} [\eta - 3(Y_{(s_i)} - 12 Y_{(mi)})]
\]

\[
(7)
\]
where \( Y_{ls} \) is the surface mass fraction, \( Y_{lm} \) the average mass fraction, \( \Gamma_l \) the liquid phase mass diffusivity coefficient, \( \rho \) the liquid density, and \( \eta \) the species mass diffusional flux at the film surface.

**Phase Equilibrium**

In a high-pressure environment, the assumption of ideal gas and liquid behavior is invalid. Consequently, the Raoult law is not appropriate to give the thermodynamical equilibrium relation between gas phase and liquid phase at the droplet or film surface. To account for the effect of non-ideal behavior at high pressure, the Peng-Robinson equation of state was used to calculate the compressibility factor and fugacity for gas phase and liquid phase. By equating species fugacities at liquid phase and gas phase, the equilibrium relation is determined.

**Property Evaluation**

Accurate property evaluations are crucial for computations of multicomponent fuel vaporization. In this study, all properties are temperature- and composition-dependent with the correction of high-pressure effect if applicable [10]. The liquid phase property is determined in the reference of average composition and temperature, and the gas phase property is evaluated using a one-third rule.

**RESULTS AND DISCUSSIONS**

All the above models have been implemented into the KIVA-3V code and verified with experimental and computational data on isolated droplets and films [4-6]. The developed method was then used to simulate air/fuel mixture preparation process for a PFI spark-ignition engine during the cold starting phase. Under the cold starting condition, the multicomponent fuel effects are the most remarkable since the fuel vaporization is incomplete and detail vaporization history is important.

The computed engine is a production 2.5L, V-6 engine that has been investigated intensively in the Spray and Engine Research Laboratory at the University of Illinois at Urbana-Champaign [7]. The fuel is composed of 15% isopentane, 20% hexane, 45% isooctane, and 20% decane by mass producing a distillation curve similar to that of a California Phase II gasoline as shown in Fig. 1.

Four cases are reported in this paper with different swirl intensity, engine speed and injection timing as summarized in Table 1. High swirl is accomplished by deactivating the secondary intake valve. Closed valve injection starts at 360° BTDC (of the intake stroke), while open valve injection starts at 0° ATDC when the intake valve is fully open. The injected spray is a solid cone spray with a spray angle of 7.5° and an SMD of 90 µm.

Computational results were first compared with an exciplex fluorescence measurement [7] for vapor in-cylinder distribution to further verify the developed method. It is worthy to mention that the experimental images are qualitative and have not been corrected for laser intensity cross-section profile and absorption of the incident laser light by the fluorescence dopants [7]. Figure 2 shows both the computed vapor density and measured vapor fluorescence image of the light component C_5H_{12} in the center plane of the cylinder at the early stage of the intake stroke (50° ATDC) for Case 1. The box in the computational image indicates imaging region of the corresponding experiment. It can be seen that the computed result agrees reasonably well with the measured one. The vapor images for the late stage of the compression stroke (310° ATDC) were shown in Fig. 3. The distribution becomes more disperse and uniform due to the mixing. The similar images for Case 2 was shown in Figs. 4 and 5. Good agreements between the computational and the experimental images were also obtained. Compared with Case 1, more fuel is accumulated in the left side of the cylinder at the early stage of the intake stroke, and the distribution becomes more uniform at the late stage of the compression stroke.

Figure 6 shows the variation of the total species vapor mass (normalized by the injection mass) versus crank angle for Case 1. The vaporization rate for all components decreases gradually with increasing crank angle before the intake valve opens. This decrease is primarily due to part of spray converting into film particles. Right before the intake valve opens, the vaporization is almost frozen because the film on the intake port wall and the valve stem reaches equilibrium with the surrounding gas. Once the intake valve opens, the intake charge motion significantly increases the vaporization rate by transporting the accumulated vapor mass and part of film mass into the cylinder. However this promotion for vaporization diminishes gradually after the intake valve fully opens. Since only little of liquid fuel enters the cylinder, the promotion for vaporization due to high-temperature created by compression is not observed. It was also shown that fuel volatility plays an important role in the vaporizing behavior. Nearly 70 percent of C_{5}H_{12} vaporized, and in contrast, little of C_{10}H_{22} vaporized. Therefore, lighter components account for higher percentage in the fuel vapor than in the injected fuel. Figure 7 shows the plot of
temporal history of in-cylinder liquid mass normalized by the injection mass. The sudden increase occurring at \( CA = 610^\circ \) is due to the closure of the intake valve and the consequent change of region definition. It is seen that more mass of heavier components is induced into cylinder. The overall percentage of each component for the in-cylinder liquid fuel is shown in Fig. 8. Compared to initial composition, the percentage of the heaviest component \( C_{10}H_{22} \) is almost doubled, while that of the lightest component \( C_{5}H_{12} \) becomes only one-third. This trend is in contrary with that for the vapor phase. These facts indicate that it is very inaccurate to use a single component fuel to represent a multicomponent fuel for cold starting computations since the in-cylinder fuel composition of either the liquid phase or the gas phase is significantly different from the injected fuel.

Figures 9 and 10 shows the variation of normalized vapor and liquid mass induced into the cylinder for four cases. The observed trends are in consistent with the experimental results [7]. The comparison between Cases 1 and 2 indicates that the higher swirl brings in more liquid and vapor into the cylinder. This is primarily due to the nearly doubled intake charge velocity, which increases the vaporization rate and the turbulence level. The entrained vapor masses for Cases 1 and 3 are close in spite of the large difference in their engine speeds (1200 rpm vs. 200 rpm). For lower speed case, the velocity and turbulence intensity in the intake port and cylinder are lower, and thus the vaporization rate in turns is slower. However, vaporization takes longer at lower engine speed. The combined effects result in engine speed having weak influence on the induced fuel mass. It is also noted that less liquid fuel mass is brought into the cylinder in the low speed case due to the intake charge motion being not strong enough to strip the film off the intake wall and the valve surface. The comparison of Cases 4 and 1 shows that open-valve injection causes more fuel vapor to be entrained into the cylinder, which is helpful for ignition and combustion. However, it also brings in much more liquid fuel most likely resulting in high hydrocarbon emissions.

CONCLUSIONS

A method for modeling multicomponent fuel effect in engines has been developed. It has the advantage of high accuracy and low computation cost. The developed method was used to simulate the air/fuel mixture preparation for a PFI spark ignition engine under the cold starting condition. It was found that the volatility of a fuel component plays an important role in determining its in-cylinder behavior. Effects of engine operating parameters (swirl intensity, engine speed and injection timing) on the in-cylinder fuel distribution were also reproduced.

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REFERENCES


Table 1. Engine operating parameters

<table>
<thead>
<tr>
<th>Case</th>
<th>Injection Timing</th>
<th>Swirl</th>
<th>Engine Speed (rpm)</th>
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<tbody>
<tr>
<td>1</td>
<td>Closed-Valve</td>
<td>Low</td>
<td>1200</td>
</tr>
<tr>
<td>2</td>
<td>Closed-Valve</td>
<td>High</td>
<td>1200</td>
</tr>
<tr>
<td>3</td>
<td>Closed-Valve</td>
<td>Low</td>
<td>200</td>
</tr>
<tr>
<td>4</td>
<td>Open-Valve</td>
<td>Low</td>
<td>1200</td>
</tr>
</tbody>
</table>

Fig. 1 Comparison of distillation curves between the used multicomponent fuel and CA Phase II gasoline

Fig. 6 The variation of species vapor mass versus crank angle for Case 1

Fig. 2 Vapor phase distribution of C₆H₁₄ at 50° ATDC of the intake (Case 1)

Fig. 3 Vapor phase distribution of C₆H₁₄ at 310° ATDC of the intake (Case 1)
Fig. 4 Vapor phase distribution of \( \text{C}_6\text{H}_{14} \) at 50° ATDC of the intake (Case 2)

Fig. 5 Vapor phase distribution of \( \text{C}_6\text{H}_{14} \) at 310° ATDC of the intake (Case 2)

Fig. 7 The variation of species in-cylinder liquid mass versus crank angle for Case 1

Fig. 8 The variation of overall mass fraction for in-cylinder liquid mass versus crank angle

Fig. 9 Comparison of induced fuel vapor mass for four cases

Fig. 10 Comparison of induced fuel liquid mass for four cases