Combustion and Spray Simulation of a GDI Engine Incorporating a Multi-Component Fuel

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Although usually simulated in combustion CFD calculations as a single-component fuel (typically iso-octane), gasoline is actually a mixture of many hydrocarbons. This paper will review the results of an in-cylinder combustion analysis of a GDI engine where the fuel is represented in both the liquid and gas phases as a multi-component mixture.

The calculations are performed using STAR-CD, a general purpose finite volume CFD code which uses the PISO algorithm (a multi-corrector variant of SIMPLE). STAR-CD incorporates a variety of physical models for sprays, turbulence, and combustion chemistry. Sprays are treated via a Lagrangian approach with sub-models for break-up, turbulent dispersion, and collision. In the analyses to be presented, initial spray distributions are formulated to match available experimental data, although STAR-CD also incorporates semi-empirical models to create distributions from available injector geometry information. The standard k-E model with wall functions is used to describe turbulence. The mesh generation process, including the description of the piston and valve motion, was automated using ICE.

When modeling a multi-component fuel with STAR-CD, two areas of the analysis need modification, sprays and combustion. The spray module of STAR-CD is already capable of handling multi-component fuels to a certain degree. As a standard feature, droplets can be composed of up to ten components, each with different specific heat, heat of vaporization, and vapor pressure characteristics and each capable of vaporizing to a different gas phase species. Other liquid parameters (density, surface tension, and viscosity) remain properties of the droplet.

In the present study, these standard features were used to describe the multi-component fuel droplets. The only new development was the creation of a user subroutine, dropro.f, to provide the component properties needed for the different fuel components. The properties chosen came from the KIVA-3V fuel library. For the remaining common droplet properties (density and so forth), the values for iso-octane were employed.

Combustion in the present study was treated with the one-equation inhomogeneous Weller flame area or flamelet model. In this model, the flame is assumed to be an infinitesimally thin sheet separating the reactants from products. Combustion chemistry enters through an empirically derived laminar flame speed expression, while the turbulence-chemistry interaction is described in a semi-empirical wrinkle factor (the ratio of the turbulent to laminar flame speed). The combustion process is tracked via a progress variable, \( c \), which is 0 in the unburnt reactant gas and 1 where combustion is complete. The variation in the progress variable is given by the following equation:

\[
\frac{\partial \Xi}{\partial t} + \nabla \cdot \rho \hat{U} \Xi - \nabla \cdot \rho D \nabla c = \frac{\rho}{\rho_u} S_u |\nabla c|
\]

where \( \Xi \) is the wrinkle factor and \( S_u \) is the laminar flame speed. The laminar flame speed is where the modifications for the multi-component fuel are incorporated into the model. However, before examining these changes, a few comments about the laminar flame speed itself are in order.

Metghalchi and Keek (2,3) found that experimentally measured laminar flame speeds could be correlated over pressure, temperature, and equivalence ratio by:

\[
S_u = S_{u0} \left( \frac{T}{T_0} \right)^\alpha \left( \frac{P}{P_0} \right)^\beta
\]

They found \( \alpha \) and \( \beta \) to be functions of equivalence ratio, \( \phi \), but independent of fuel type:

\[
\alpha = 2.18 - 0.8 (\phi - 1)
\]

\[
\beta = -0.16 + 0.22 (\phi - 1)
\]

The reference flame speed was also found to be a function of equivalence ratio:

\[
S_{u0} = B_m + B_2 (\phi - \phi_m)^2
\]

but the B coefficients were found to be fuel dependent (\( \phi_m \sim 1.1 \) for most hydrocarbons).
Unfortunately, the polynomial expression used by Metghalchi and Keek in their correlation leads to negative flame speeds at high and low equivalence ratios. While it is possible to arbitrarily correct this behavior, a more elegant solution can be obtained by switching the form of the expression. Gülder (4) proposed a correlation which does not exhibit the negative flame speed behavior at high and low equivalence ratios (see Figure 1):

\[ S_{\nu_e} = \omega \phi^n e^{-\xi \phi - \zeta^2} \]

Of course, the question is which behavior is accurate. As Figure 1 shows, the Metghalchi and Keek data is of little utility here, since it is very limited in equivalence ratio range. However, where there is data available (see Figure 2), the Gülder approach seems more accurate.(5)

Figures 1 and 2 point out the limited availability and extent of experimental laminar flame speed data. While data for fuels such as propane and iso-octane is readily available, data for other hydrocarbons is very limited or nonexistent. However, the data that does exist suggests that variations in flame speed between the various hydrocarbons generally correlate with molecular weight, as shown in Figure 3. (3,6,7) The exception is Toluene, which has a flame speed similar to iso-octane but a Bower molecular weight.

Having decided on the form of the laminar flame speed correlation and determined a relationship to generate the flame speeds for the component fuels, %II that remains is to determine a means of extending the Weller model to multi-component fuels. We assert that the laminar flame speed for a mixture of fuels can be found as the mixture fraction-weighted sum of their individual flame speeds at the same overall mixture fraction.

Results show the fuel vapor component mass fractions as a function crank angle (Figure 4), as well as fuel vapor and temperature contours at a cross-section through the center of the chamber (Figures 5 and 6). Comparisons are drawn between single- and multi-component fuel analyses.

Figure 1. Octane Laminar Flame Speed Correlations.

Figure 2. Propane Laminar Flame Speed Correlations.
Figure 3. Laminar Flame Speed vs. Molecular Weight.

Figure 4. Multi-Component Fuel Vaporization Histories for a GDI Engine.
FIGURE 5: TOTAL FUEL MASS FRACTION CONTOURS FOR A GDI ENGINE SECTION THROUGH CYLINDER CENTERLINE
FIGURE 6: TEMPERATURE CONTOURS FOR A GDI ENGINE
SECTION THROUGH CYLINDER CENTERLINE