Estimating the composition of the residual gases for use in a multi-cycle engine model

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Introduction

- Detailed chemical kinetic simulations were run using the Ignition Progress Variable (IPV) model under constant-volume adiabatic conditions in ANSYS Chemkin-Pro. [1]
- The composition of the residual has been estimated using reduced tabulated results from detailed chemical kinetic simulations.

Background

- Dilute spark-ignition (SI) engine operation decreases fuel consumption and reduces emissions.
- Increased dilution is limited by the occurrence of incomplete combustion events (i.e. misfires and partial burns). A dilution limit is reached when these events occur at a predetermined level.
- The cycle-to-cycle dynamics at the dilution limit are primarily caused by the feed-forward mechanism present in the residual gases.[2]
- A multi-cycle engine model is being used to better understand the cycle-to-cycle dynamics at the dilute limit. To successfully do this, variations in the residual must be adequately captured at a low computational cost.

IPV model

The results presented are for the following initial conditions:

- Equivalence ratio of 0.7
- Initial Temperature 600 K
- Initial Pressure 30 bar

The progress variable defines the completeness of combustion. Chemkin-Pro uses the definition by Bo et al.[3] to define the progress variable as:

$$c(t) = \frac{h_{298\,\mathrm{K}}(t) - h_{298\,\mathrm{K}}(t = t_0)}{h_{298\,\mathrm{K}}(t = t_{end}) - h_{298\,\mathrm{K}}(t = t_0)}$$

where $h_{298\,K}$ is the enthalpy of the mixture at 298 K. $c = 0$ corresponds to unburned conditions and $c = 1$ corresponds to equilibrium conditions.

Lookup Table Formulation

- Species of interest for this study are CO_2, H_2O, N_2, O_2, CO, H_2, and IC_8H_{18}.
- Lookup tables (LUTs) are a function of the progress variable and equivalence ratio.
- The progress variable can be redefined using a different parameter. This parameter must be monotonic and represent the entire reaction.[4]
- The progress variable is redefined using some linear combination of major species.[5]
- Nontabulated species are solved for using an atom balance. The number of atoms are assumed to be constant within a cycle.
- The mass fraction of N_2 is constant for a given equivalence ratio thus only six species are unknown.

Different linear combinations of the species of interest that are found in the literature were tested.[4-6] The progress variable for all combinations were calculated using:

$$c = \frac{x_c - x_c^0}{x_c^{eq} - x_c^0}$$

where x_c^0 and x_c^{eq} are the initial and equilibrium value of x_c.

The atom balances used to solve for the untracked species are:

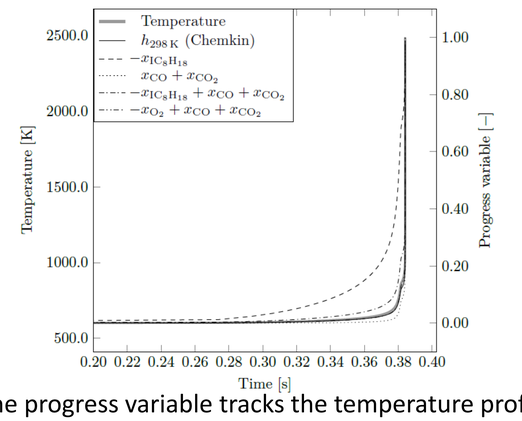
$$n_{\mathrm{carbon}} = 8\frac{x_{\mathrm{IC_8H_{18}}}}{MW_{\mathrm{IC_8H_{18}}}} + \frac{x_{\mathrm{CO}}}{MW_{\mathrm{CO}}} + \frac{x_{\mathrm{CO_2}}}{MW_{\mathrm{CO_2}}}$$

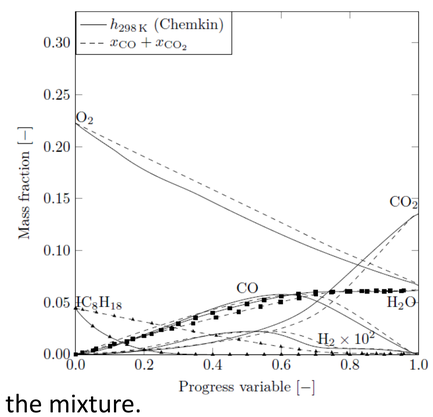
$$n_{\mathrm{hydrogen}} = 18\frac{x_{\mathrm{IC_8H_{18}}}}{MW_{\mathrm{IC_8H_{18}}}} + 2\frac{x_{\mathrm{H_2O}}}{MW_{\mathrm{H_2O}}} + 2\frac{x_{\mathrm{H_2}}}{MW_{\mathrm{H_2}}}$$

$$n_{\mathrm{oxygen}} = \frac{x_{\mathrm{CO}}}{MW_{\mathrm{CO}}} + 2\frac{x_{\mathrm{CO_2}}}{MW_{\mathrm{CO_2}}} + \frac{x_{\mathrm{H_2O}}}{MW_{\mathrm{H_2O}}} + 2\frac{x_{\mathrm{O_2}}}{MW_{\mathrm{O_2}}}$$

where n is the number of carbon, hydrogen, or oxygen atoms in the mixture, x_i and MW_i are the mass fraction and molecular weight of species i.

Results





- The progress variable tracks the temperature profile of the mixture.
- CO and CO_2 should be included to define the progress variable. This still leaves three equations with four unknowns.
- A third species must be tracked. H_2 was used as the third known species.
- The detailed chemical mechanism estimates fuel depletes before combustion is complete because the fuel breaks down into intermediate fuel species and lighter hydrocarbons.

Conclusions

- The completeness of combustion was redefined using a linear combination of the mass fractions of CO and CO_2.
- The mass fractions of CO, CO_2, and H_2 were tabulated from detailed chemical kinetic simulations.
- Remaining species of interest were found by balancing the number of carbon, hydrogen, and oxygen atoms in the mixture.
- While only one equivalence ratio is presented here, the same trends are present at different equivalence ratios.

Future Work

- The lookup tables and atom balance will be implemented into the multi-cycle engine model to capture variations in the residual from cycle-to-cycle.
- The mass fraction burned and equivalence ratio from the current cycle of the multi-cycle engine model will be used as the progress variable and equivalence ratio of the lookup tables.

References

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