An empirical modeling approach for the ignition delay of fuel blends based on the molar fractions of fuel components

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ABSTRACT

An empirical ignition delay model has been developed for the fuel blends of isooctane, n-heptane, toluene and ethanol based on their molar fractions in the stoichiometric condition. The model employs traditional Arrhenius type correlation and cool-flame temperature rise correlations to describe the negative temperature coefficient (NTC) region for the fuel blends. The overall ignition delay of a fuel blend is correlated with individual ignition delay information based on the molar fraction of the fuel component in the mixture. The proposed model is successfully validated against the published experimental ignition delay data using various binary, ternary and quaternary fuel blends of isooctane, n-heptane, toluene and ethanol.

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1. Introduction

Engine knock in spark ignition (SI) engines is characterized by the noise that is transmitted through the engine structure when auto-ignition of unburned end gas ahead of flame front occurs [1]. Knock in SI engine is one of factors that limits higher compression ratio, spark advance, and intake boost level. An accurate and efficient numerical engine combustion model with a capability of predicting the auto-ignition phenomenon can be a powerful engine development tool during the early engine development stage by reducing prototype based experimental development cost and time. Auto-ignition is affected by the fuel properties as well as the cylinder temperature and pressure evolution during the combustion process. Since commercially available fuel is a complex blend of hydrocarbons, the characteristics of the auto-ignition of the fuel is strongly influenced by its composition. Ideally, chemical kinetics models would provide good prediction, but current researches on these chemical kinetics models are only available for a limited number of fuel components. In addition, the complexity and huge computational time make it impractical to incorporate them directly into an engine system level simulation. Reduced and skeletal chemical kinetics models are more suitable for this type of application, but they still need calibration using experimental data and computation load can be still problematic depends on the type of simulation. Therefore, empirical auto-ignition correlations have been developed and widely used for variety of engine system simulations.

The auto-ignition of hydrocarbon fuel is governed by fundamental chemical reaction principles and the ignition delay can be described by an Arrhenius type correlation. Livengood and Wu [2] developed the classic Knock-Integral approach using the data from a rapid compression machine to predict the time of knock occurrence. In their model, the auto-ignition is presumed to occur when the integral of the inverse of ignition delay correlation becomes unity over a period of time using the pressure and temperature history of the fuel–air mixture in the cylinder. The knock integral method has been widely used for knock predictions due to its concept of calculating ignition delay when charge conditions are not steady state [3–5]. An adaptable correlation developed by Douaud and Eyzat [6] includes octane number to an ignition delay correlation and had been validated for various commercially available fuels:

$$\tau = 17.68(ON/100)^{3.402}p^{-1.7}\exp(3800/T) \tag{1}$$

where τ is ignition delay (ms), p and T are pressure (atm) and temperature (K), and ON is the octane number. This single stage Arrhenius type model was validated by Kim and Ghandhi [7] by comparing the simple correlation model with detailed chemical kinetics model in predicting knock. They concluded that the Douaud

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Nomenclature

Notation

$[A]$	concentration of air (mol/cm^3)
$[F]$	concentration of fuel (mol/cm^3)
A	air
C	calibration coefficient
C_{CP}	coefficients for specific heat correlation
C_p	constant pressure specific heat (J/K)
F	fuel
K	reaction rate constant
N	total number of pure components in the fuel blend
n	mole number
ON	octane number
p	pressure (bar)
P	product of pre-ignition reaction
R	universal gas constant (J/mol K)
T	temperature (K)
t	time (ms)
V_{FA}	volume of fuel air mixture (cm^3)
Y	molar fraction
α	precursor species for ignition
β	proportionality constant

v_a	volume fraction of alcohol
τ	characteristic ignition delay (ms)
τ_b	ignition delay of blend fuel (ms)
τ_c	cool flame ignition delay (ms)
τ_{hCF}	exothermic reaction delay at post cool flame condition (ms)
τ_{hi}	exothermic reaction delay at pre-cool flame condition (ms)
ϕ	equivalence ratio
ω	reaction rate (mol/s)

Subscripts

b	blend
CF	evaluated at post cool flame condition
cc	coefficient correlation
F	fuel
i	evaluated at initial condition
ign	evaluated at ignition
j	fuel component in blend
$MEOH$	methanol
PRF	primary reference fuel

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and Eyzat Arrhenius correlation is as accurate as the chemical kinetics model in some specific regions. However, it is not able to describe the two-stage ignition and deflagration with a single Arrhenius type correlation. It does not capture the cool flame phenomenon [8], which paraffin class fuels with the form of $C_nH_{2n+2}(n > 2)$ exhibit during the ignition delay period. Cool flame phenomena are usually associated with so called negative temperature coefficient (NTC) behavior of the reaction rate in low and intermediate temperature regions, and are characterized by an abrupt temperature rise after the pre-cool flame delay period. An example of such ignition delay is shown in Fig. 1. The cool flame region is shown in the upper right corner of the plot, where two-stage ignition with cool flame phenomenon takes place. The cool flame releases heat which increases temperature and such effect shortens overall ignition delay. In the intermediate temperature region, an evidence of the NTC behavior can be observed. As initial temperature increases, cool flame reaction slows down and eventually shuts off [9]. Therefore, cool flame temperature rise effect degrades and ignition delay becomes longer as initial temperature

increases. In the high temperature region, ignition delay shows positive temperature coefficient behavior again.

In order to model the two-stage ignition and capture the NTC region, Yates and Viljoen [11] developed an Arrhenius type two stage ignition delay model. The model was calibrated with results from more than 1500 detailed chemical kinetics simulations to fit a wide range of temperatures, pressures, fuel–air equivalent ratios and octane numbers. It predicts the time delay before the cool flame, abrupt temperature rise and overall ignition delay for primary reference fuel (PRF) and methanol blends by employing the Knock-Integral method explained in Livengood and Wu [2] and expanding it to a two-stage integration by integrating different correlations in different temperature regions. This model describes the trend of the NTC region in a reasonable manner. Iqbal et al. [12] also employed the model and calibrated it using detailed CHEMKIN chemical kinetics model for toluene reference fuel 91 (TRF91: 53.8% isooctane, 13.7% *n*-heptane, 32.5% toluene). The fuel is regarded as a better representative of the gasoline than PRF because TRF exhibits similar octane sensitivity as commercial gasoline does. In their research, the octane number was not used but exhaust gas recirculation (EGR) rate was taken into account.

He et al. [13] and Walton et al. [14] incorporated oxygen fraction and fuel air equivalent ratio in their correlation for the ignition delay of isooctane. Then Goldsborough [15] improved it based on the functional behavior exhibited by a detailed chemical kinetics to capture the NTC region. The correlation employs a single Arrhenius type power law formulation including equivalence ratio, temperature, pressure, and oxygen concentration. The coefficients of the Arrhenius type correlation are expressed as a combination of two quadratic terms with respect to temperature and pressure to calculate the NTC behavior. Syed et al. [16] developed a simple correlation for the ignition delay of gasoline-ethanol blend fuel. The model was calibrated using the result from a CHEMKIN closed homogeneous reactor model with a validated semi-detailed chemical kinetics mechanism consisting of 142 species and 672 reactions. It employed pre-defined coefficient tables corresponding different temperatures, equivalence ratios and ethanol volume fractions in order to describe appropriate ignition delay behaviors in wide range of conditions.
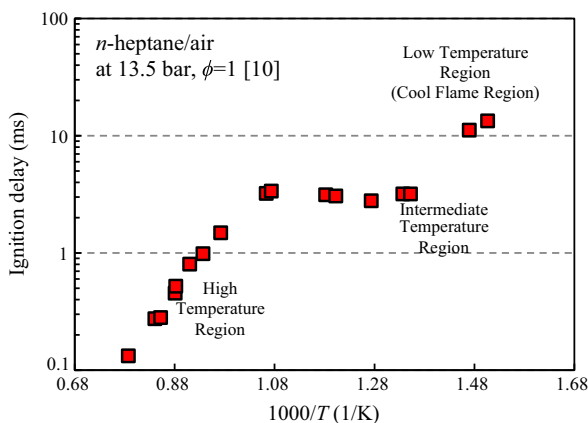

Fig. 1. Shock tube ignition delay versus reciprocal temperature profiles extracted from Ciezki and Adomeit [10] for *n*-heptane with stoichiometric fuel/air equivalent ratio.