

An alternative approach to accommodate detailed ignition chemistry in combustion simulation



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ABSTRACT

In the current work, we utilize a recently developed staged Livengood–Wu (L–W) correlation to evaluate and predict the two-stage ignition behaviors of different primary reference fuels (PRFs) under homogeneous reciprocating engine conditions, to demonstrate its capability in capturing detailed ignition kinetics in combustion simulation. Based on the understandings of the global and detailed kinetics of low-temperature chemistry, simplified Arrhenius-based global expressions were developed for both ignition stages, and a linear correlation was applied for the cool flame temperature rise at the end of the first stage, for PRFs with various octane number (ON) 0, 20, 60 and 87 under constant volume conditions. For their performance under homogeneous charge compression ignition (HCCI) conditions, it is shown that for the same engine speed, the inlet temperature range allowing for two-stage ignition shrinks with increased ON numbers, and eventually two-stage ignition turns into single-stage ignition with sufficiently high ON numbers. Based on the ignition database, the combustion phasing for all PRFs under a wide HCCI operation range are predicted with the staged L–W integral method with satisfactory accuracy, including the first- and second-stage ignition timing as well as the cool flame temperature rise. The sensitivities of each of the engine operation parameters are successfully captured, further demonstrating the applicability of the staged L–W method for realistic fuels with low temperature chemistry and its potential applications for engine combustion control. This study also provides an alternative approach of accommodating low temperature ignition kinetics in combustion simulation, especially useful for those under variable thermodynamic conditions.

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1. Introduction

Auto-ignition plays a crucial role in the operation of internal combustion engines due to its close relation to knock onset in spark-ignition (SI) engines and control of combustion phase in compression ignition (CI) engines, albeit their distinctive combustion strategies. To interpret auto-ignition and predict the occurrence of knock in engines, by considering the ignition delay time $\tau(P, T)$ as a measure of the mixture reactivity with given thermodynamic conditions (pressure P and temperature T), Livengood and Wu [1] proposed a predictive, integral method based on the accumulation of a critical concentration of the chain carriers to correlate the auto-ignition timing in internal combustion (IC) engines, τ_{ICE} , with those in rapid compression machines (RCMs) by integrating over the thermodynamic path using the formula $1 = \int_0^{\tau_{ICE}} \frac{dt}{\tau(T(t), P(t))}$. This method, hereafter referred to as the conven-

tional L–W correlation, has been widely used in the prediction and correlation of auto-ignition in SI [2], HCCI [3–4] and RCCI [5] engines due to its simplicity and accuracy, especially for cases where the ignition delay can be well described by the single-step Arrhenius kinetics [6–8] or described by other analytical expressions [9]. This idea not only decouples the thermodynamic conditions from the chemical kinetics, but also makes the prediction of engine ignition timing feasible by simply using the inverse of ignition delay as a general indicator for chemical reactivity.

It is well recognized that during auto-ignition of fuel–oxidizer systems, the ignition response can vary *non-monotonically* with the global parameters such as pressure and temperature due to the variation of controlling chemistry. A featured example could be the negative temperature coefficient (NTC) response in the low-to intermediate-temperature range for general large hydrocarbon fuels, during which the entire auto-ignition process proceeds in two stages, with the first controlled by low-temperature chemistry involving large oxygenated species, and the second controlled by intermediate-to-high temperature chemistry involving smaller species. The change of the thermodynamic states due to heat

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release as well as the different characteristic chain carriers during the two-stage auto-ignition is fundamentally beyond the capability of the original L–W correlation. Consequently, it has been demonstrated that such low temperature chemical reactivity plays an essential role in the novel class of low temperature flames [10], evolution of engine combustion modes [11], control of engine combustion phases [12] and the development of novel engine combustion strategies [13]. Therefore, it would be helpful to further extend the original L–W correlation to account for such effects, especially for the two-stage ignition phenomena within the NTC regime [14,29]. Actually, with the recent developments such as engine inlet boost and downsizing [15], the elevated in-cylinder pressure inevitably promotes the low-temperature chemistry even for high-octane gasoline fuels, which therefore necessitates the needs of a simple prediction method for engine ignition timing accommodating realistic chemistry and two-stage ignition.

A few worthwhile studies have attempted such a two-stage L–W based method, albeit with mixed success. Yates et al. [16,17] proposed a global empirical model for the auto-ignition delay considering the cool flame temperature rise for constant volume auto-ignition of alcohol-PRF (Primary Reference Fuel) blends, which nevertheless involves many empirical parameters to be tuned. Colin et al. [18] presented a method for two-stage combustion based on tabulated reaction rates including cool flame fuel consumption and ignition delay, limited by high-dimensional reaction rate tables. Hernández et al. [19] proposed and tested alternative forms of staged L–W model of *n*-heptane, which unfortunately were either unable to predict two-stage ignition delay due to the difficulty in resolving the cool flame state, or show poor accuracy. A recent work by Pan et al. [20] has developed a staged L–W correlation to satisfactorily capture the ignition delay in both stages of the two-stage ignition, as well as the cool flame temperature increment in the operation of HCCI engines. In their approach, simple physics-based correlations are developed to separately describe the constant volume ignition delays of the first and second stages as well as the temperature increase at the end of the first stage. Based on this database, two separate L–W integrals are further proposed to successfully predict the ignition timings of both stages for *n*-heptane and DME, two typical fuels exhibiting NTC.

In this work, the staged L–W correlation is further extended to study and predict the behaviors of PRFs with different octane numbers (ONs) and engine operation conditions, to further justify its applicability to fuel mixtures with various chemical reactivities and engine operations. Meanwhile, ignition database for selected PRFs has been reported and kinetic features of different PRFs under extensive engine conditions are investigated and accentuated. This work shall be a useful intermediate step to eventually predict and control the performance of advanced IC engines for realistic fuel blends with realistic chemistry, especially under boosted, downsized and increased compression ratio conditions where the low temperature chemistry is promoted [31,32].

On the other hand, it should be noted that when the traditional integral approach was introduced, the field of combustion kinetics of hydrocarbon did not actually exist. Now that substantial progress has been made by kinetic model developers for various simple hydrocarbons and surrogate models for practical fuels. However, due to the large size or unavailability of the kinetic model for multicomponent practical fuels, as well as the complex nature of flow, 3D direct numerical simulation (DNS) of many combustion problems including the modeling of engine combustion is still unfeasible. Therefore, the staged L–W approach could serve as an alternative way to indicate the local ignitability for both cool flame and hot ignition. For example, current efforts are being conducted combining the G-equation for turbulent flame propagation and the staged L–W integral at a few markers in the flow field to simulate spark-ignition engine combustion and predict engine

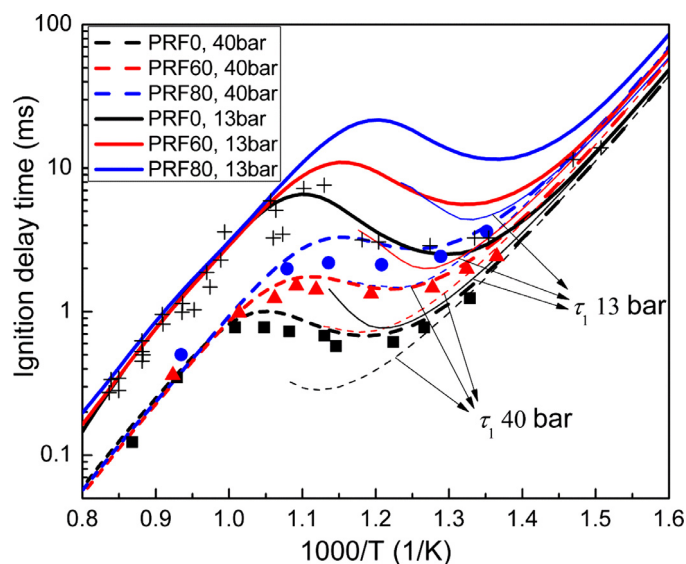


Fig. 1. Adiabatic constant volume simulation for total and first-stage ignition delay time for different PRFs under 13 and 40 bar. Solid lines represent 13 bar, and dashed lines represent 40 bar. Bold lines show total ignition delay time and slim lines show the first-stage ignition delay. Circles, triangles and squares are experimental data [24] for PRF 80, 60, 0 at 40 bar respectively; black cross symbols are experimental data of PRF0 at 13.5 bar [23,24].

knock with much less efforts and reasonable accuracy. Another highlight is that the motivation of the original L–W is to correlate ignition timing obtained from different combustion facilities, such as in RCM and IC engines. The previous L–W cannot accommodate the low temperature chemistry (LTC), which has substantial effect for a wide range of engine operation conditions and other facilities with variable thermodynamic conditions (e.g., miniature shock-tube, constant volume combustion bomb, etc). Therefore, the current method is very useful for cross validation among data obtained from different facilities with LTC. In summary, the staged L–W method provides an alternative way for auto-ignition prediction in general 3D combustion modeling, and it is useful to achieve experimental data cross-validation in experimental facilities with variable thermodynamic conditions.

2. Model validation and ignition database construction

The chemical kinetic mechanism for the PRFs used in this work was developed and validated by Mehl et al. [21], including 1387 species and 5739 reactions, based on which auto-ignition simulations are performed with the SENKIN code in the Chemkin II package [22] and further validated against available experimental data [23,24] for three different stoichiometric PRFs/air mixtures under 13 and 40 bar, as shown in Fig. 1. For these calculations, the instant of the local maximum temperature rise rate is defined as the indicator of ignition for each stage. Four observations could be achieved from Fig. 1: (1) with increased ON, the total ignition delay largely increases in the NTC regime and slightly increases in the low temperature regime, while negligible change is shown in the high temperature regimes, implying higher chemical reactivity of *n*-heptane in low to intermediate temperature regimes; (2) with increased fraction of iso-octane for higher ON PRFs, the NTC regime shifts towards lower temperatures at the same pressure; (3) for all the PRFs studied, with increased pressure, ignition delay time decreases and the NTC regime shifts towards higher temperatures; (4) with decreased ON and/or increased pressure, two-stage ignition is extended to higher temperatures as indicated by the shift of the minimum of the first stage ignition delay. These behaviors summarized here have also been noted by previous modeling

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