



# The structure and propagation of laminar flames under autoignitive conditions



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## ABSTRACT

The laminar flame speed  $s_l$  is an important reference quantity for characterising and modelling combustion. Experimental measurements of laminar flame speed require the residence time of the fuel/air mixture ( $\tau_f$ ) to be shorter than the autoignition delay time ( $\tau$ ). This presents a considerable challenge for conditions where autoignition occurs rapidly, such as in compression ignition engines. As a result, experimental measurements in typical compression ignition engine conditions do not exist. Simulations of freely propagating premixed flames, where the burning velocity is found as an eigenvalue of the solution, are also not well posed in such conditions, since the mixture ahead of the flame can autoignite, leading to the so called “cold boundary problem”. Here, a numerical method for estimating a reference flame speed,  $s_R$ , is proposed that is valid for laminar flame propagation at autoignitive conditions. Two isomer fuels are considered to test this method: ethanol, which in the considered conditions is a single-stage ignition fuel; and dimethyl ether, which has a temperature-dependent single- or two-stage ignition and a negative temperature coefficient regime for  $\tau$ . Calculations are performed for the flame position in a one-dimensional computational domain with inflow-outflow boundary conditions, as a function of the inlet velocity  $U_I$  and for stoichiometric fuel–air premixtures. The response of the flame position,  $L_f$ , to  $U_I$  shows distinct stabilisation regimes. For single-stage ignition fuels, at low  $U_I$  the flame speed exceeds  $U_I$  and the flame becomes attached to the inlet. Above a critical  $U_I$  value, the flame detaches from the inlet and  $L_f$  becomes extremely sensitive to  $U_I$  until, for sufficiently high  $U_I$ , the sensitivity decreases and  $L_f$  corresponds to the location expected from a purely autoignition stabilised flame. The transition from the attached to the autoignition regimes has a corresponding peak  $dL_f/dU_I$  value which is proposed to be a unique reference flame speed  $s_R$  for single-stage ignition fuels. For two-stage ignition fuels, there is an additional stable regime where a high-temperature flame propagates into a pool of combustion intermediates generated by the first stage of autoignition. This results in two peaks in  $dL_f/dU_I$  and therefore two reference flame speed values. The lower value corresponds to the definition of  $s_R$  for single-stage ignition fuels, while the higher value exists only for two-stage ignition fuels and corresponds to a high temperature flame propagating into the first stage of autoignition and is denoted  $s'_R$ . A transport budget analysis for low- and high-temperature radical species is also performed, which confirms that the flame structures at  $U_I = s_R$  and  $U_I = s'_R$  do indeed correspond to premixed flames (deflagrations), as opposed to spontaneous ignition fronts which do not have a unique propagation speed.

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## 1. Introduction

The laminar flame speed  $s_l$  is an important quantity in combustion which provides a unique reference value for the rate of unstretched laminar flame propagation at a given thermochemical state. The validation of chemical kinetic models, the analysis of

scientific measurements, and the engineering design process all benefit from accurate measurements of  $s_l$  at relevant conditions. Experimental measurements of  $s_l$  require that the ignition delay time of the fuel/air mixture  $\tau$  is much longer than the corresponding mixture residence time  $\tau_f$ , which is not satisfied for autoignitive conditions where  $\tau$  becomes very small. For conditions which have a sufficiently large  $\tau$ , numerical calculations of  $s_l$  are usually performed for a freely propagating, adiabatic, un-stretched flame moving into an un-reacted upstream mixture [1]. With this

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approach,  $s_f$  is an eigenvalue solution, corresponding to the inlet velocity. However, at autoignitive conditions, which exist for many combustion devices such as internal combustion (IC) engines, this method does not produce a unique solution.

The “cold boundary problem” is a long recognised concept [2] that identifies the contradiction between mathematical models for steady flame propagation and the underlying physical properties of combustible mixtures. Flammable mixtures have a finite ignition delay time,  $\tau$ , and therefore the reactant mixture is changing ahead of the flame and a steady-state solution does not, in principle, exist [3]. In practice, for a sufficiently cold reactant mixture,  $\tau$  is essentially infinite compared to the characteristic flame time  $\tau_f$  and a steady-state may be measured from experiment or calculated from numerical simulation. However, this approach fails where the reactant mixture is not sufficiently cold and  $\tau \approx \tau_f$ , leading to domain size (residence time) dependent solutions.

Nonetheless, calculations of  $s_L$  have been performed for steady [4–8] and transient [9–11] premixed flames at autoignitive conditions. The transient calculations approximate  $s_L$  by initiating a hot-spot that transitions to a flame and the speed of the flame front with respect to the unburnt mixture is taken to be  $s_L$ . While this provides an estimate of  $s_L$ , this method cannot define a unique value as the result depends upon many factors including the details of the initial hot-spot and the duration of front propagation used to estimate  $s_L$ . Steady state calculations of  $s_L$  at autoignitive conditions using solvers such as, e.g. PREMIX [12] or Cantera [13], usually do not address the cold boundary problem, and so the interpretation of those solutions is unclear. However, recently Sankaran performed a study of freely propagating laminar hydrogen flames at autoignitive conditions using Cantera [6] that did address this issue. In that study, the dependence of the solution on the domain size was used to investigate transitions in the flame structure. For sufficiently long domains, the steady-state solution was an autoignition front due to the long residence times. For sufficiently small domains, a premixed flame was observed with little chemical reactions ahead of the front. The results highlighted the effect of domain size on the eigenvalue problem at autoignitive conditions, and explored the possible flame structures that may arise for a single-stage ignition fuel.

The distinctions between deflagrative flames (in which conduction and diffusion play a major role in flame propagation) and spontaneous ignition fronts (in which propagation is driven by gradients of ignition delay time) [14] have been numerically investigated for constant volume reactors [4,7–10,15–25]. These studies considered the transient ignition process subject to temperature [4,8,9,15–17,19,21–23,25] and/or velocity [8,16,21,22,25] and/or composition [17,19,21,24] fluctuations in physical space. For instance, temperature fluctuations dictate spatial gradients in  $\tau$ , which control the speed of spontaneous ignition fronts [9,14,15], such that higher (lower) temperature fluctuations lead to slower (faster) spontaneous ignition front speeds and a lesser (greater) contribution to the overall ignition compared to the contribution from deflagrations. This picture is modified by turbulence, which produces a competition between mixing and chemistry and a regime diagram has been proposed to explain the various combustion modes that may occur [8,22]. Many other insights have been gained from these studies, however, the present study focusses on the behaviour of steady-state flames within a spatially developing domain and not on the temporally evolving ignition process.

IC engines operate at elevated pressures and temperatures. At these conditions, the distinction between autoignition and flame propagation [14] is physically meaningful from a modelling and design perspective, but very challenging to quantify due to the extreme conditions. For instance, a critical parameter in diesel combustion is the lift-off length (LOL) which affects the mixing and

pollutant formation processes [26]. The prediction of the LOL depends upon the underlying method of flame stabilisation and so distinguishing between autoignition and flame propagation is important. However, in the absence of resolved flame measurements, it is difficult to distinguish between these modes of combustion. Reference flame speed estimates at these conditions would place some bounds on the possible turbulent flame speeds, and may therefore assist in distinguishing between ignition and flame propagation stabilisation modes.

At IC engine conditions, the fuel may exhibit single or two-stage autoignition depending on the exact thermochemical state. A single stage ignition fuel, such as ethanol ( $C_2H_5OH$ ) (at the conditions considered in the present study), has a monotonic decreasing relationship of  $\tau$  with the initial mixture temperature. For two-stage ignition fuels, such as dimethyl ether ( $CH_3OCH_3$ ) (DME) considered in the present study, and *n*-dodecane which is widely used in the engine combustion community for diesel-relevant conditions [27,28], low-temperature chemistry (LTC) leads to a first-stage of autoignition that is distinct from the second, main stage of autoignition due to high-temperature chemistry (HTC). The temperature-dependent interaction between the first- and second-stages of autoignition produces a regime of negative temperature coefficient (NTC) behaviour for  $\tau$ .

Many recent studies have been performed for DME at NTC conditions [7,17,18,29–34]. In particular, the behaviour of the LTC has received much attention. Under certain conditions, the LTC can establish a cool flame which propagates like a wave. Stable premixed [32] and nonpremixed [29] cool flames have been experimentally observed and numerical simulations have investigated the complex transitions and flame structures that can exist due to the interactions between the cool flame and the high-temperature flame [7,30,31,34–36]. These interactions may be important for IC engines, as the cool flame can influence the ignition delay time and most reactive mixture location for diesel combustion [36–39] and engine knock in spark ignition engines, e.g., Refs. [7,40,41].

It has been shown that the propagation of partially premixed DME flames at IC engine conditions can lead to a range of possible flame structures depending upon the oxidiser temperature,  $T_{OX}$  [30], and inlet velocity,  $U_I$  [31]. At lower  $U_I$  and lower  $T_{OX}$ , conventional tribrachial (triple) flames are observed that are stabilised primarily by premixed flame propagation (deflagration) and flow divergence due to gas expansion. As  $U_I$  and  $T_{OX}$  increase, additional branches appear upstream of the main tribrachial flame due to the first-stage of autoignition (due to LTC) and/or the second stage of autoignition (due to HTC); these polybrachial flames are stabilised by a combination of autoignition and flame propagation [30,31]. For sufficiently high  $T_{OX}$  or  $U_I$ , the flame is stabilised purely by autoignition. In other words, the flame propagation speed is directly related to the mode of combustion and it is ambiguous as to how to define a reference value. Recent DNS studies of turbulent, partially premixed combustion at NTC conditions have measured the displacement speed of polybrachial edge flames [11,35,42]. Minamoto and Chen observed that the partially reacted mixture ahead of the high-temperature flame (due to LTC) affects the estimated flame speed, similar to the analysis for single stage ignition fuels with temperature non-uniformities [9,10] and experimental observations of a turbulent slot flame featuring two-stage ignition chemistry [5].

Experimental studies have been performed on laminar partially premixed flame stabilisation for *iso*-octane [43] and *n*-heptane [44] fuels at elevated temperatures and atmospheric pressure. In those studies, measurements of the flame height from the inlet,  $L_f$ , versus  $U_I$  were presented which, alongside visualisations of the flame structure, identified transitions from edge-flame propagation to autoignition with increasing  $U_I$ . For *iso*-octane, plots of  $L_f$  versus  $U_I$  identified transitions from burner-stabilised, to edge-flame

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