DETERMINATION OF LAMINAR FLAME SPEED OF DIESEL FUEL FOR USE IN A TURBULENT FLAME SPREAD PREMIXED COMBUSTION MODEL

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ABSTRACT

One of the key challenges facing diesel engine system modelers lies in adequately predicting the fuel burning rate profile given the direct relationship between energy release and key performance parameters such as fuel economy, torque, and exhaust emissions. Current state-of-the-art combustion sub-models employed in such system simulation codes rely heavily on empiricism and successful application of such sub-models for new engine designs is highly dependent on past experience with similar combustion systems. One common approach to address this issue is to expend great effort choosing associated empirical coefficients over a range of similar combustion system designs thus improving the potential predictive capability of a given empirical model. But, continual combustion system development and design changes limit the extrapolation and application of such generic combustion system dependent coefficients to new designs due to various reasons including advancements in fuel injection systems, engine control strategy encompassing multiple injections, and combustion chamber geometry.

In order to address these very difficult challenges, an extensive effort has been applied toward developing a physically based, simplified combustion model for military-relevant diesel engines known as the Large Scale Combustion Model (LSCM). Recent effort has been spent further refining the first stage of the LSCM two stage combustion model that is known as the premixed phase sub-model. This particular sub-model has been compared with high-speed cylinder pressure data acquired from two relevant direct injection diesel engines with much success based on a user defined parameter referred to as the laminar flame speed by the combustion community. It is a physically significant parameter that is highly dependent on local temperature, pressure, and oxygen concentration but little experimental effort has been spent determining its behavior for diesel fuel due to ignition constraints. This submission will discuss one approach of indirectly determining this key combustion parameter.

INTRODUCTION

Diesel combustion modeling is difficult from a fundamental perspective due to the lack of three-dimensional understanding thus making simplified (zero- or quasi-dimensional) approaches even more difficult. The engine community has seen a tremendous advancement in understanding and predictive capability throughout the last fifty years and especially since the 1970's given the advent of supercomputers. One of the earliest attempts to model combustion in a diesel-like environment was based on a droplet evaporation control approach (Tanasawa, 1953) that utilized previous work focused on establishing droplet size distribution functions (Probert, 1946). Shortly afterward, this work was extended to include the effect of the injection rate on droplet evaporation (Austen and Lyn, 1961; Lyn, 1962) thus directly accounting for the role of the fuel injection event in the combustion process. This well known model is commonly referred to as the 'triangular burning rate law'. It was subsequently recognized by various researchers that inclusion of a semi-predictive combustion model would be very valuable within the context of an overall engine system model (Cook, 1963; McAulay et al., 1965; Cook, 1965; Nagao et al., 1967) and thus much effort has been spent by the engine community in developing more predictive heat release models. In the late 1960's one of first comprehensive models was developed that included coupled global evaporation, mixing, and kinetics effects (Shipinski et al., 1968, 1970).

At the onset of the 1970's emissions became an additional focus of such combustion model development efforts. The engine community subsequently developed chemically kinetic and mixing controlled combustion models (Whitehouse and Way, 1970, 1971), bulk mixing rate submodels (Grigg and Syed, 1970; Khan et al., 1971), and thermodynamic multi-zone models (Bastress et al., 1971; Shahed et al., 1973, 1975; Hodgetts and Shroff, 1975; Chiu et al., 1976; Hiroyasu and Kadota, 1976; Maguerdichian and Watson, 1978). These efforts were fundamental in establishing the basis for today's multi-zone and bulk mixing combustion models that have been fine tuned throughout the last twenty-five years through careful development of air-fuel mixing submodels (Dent and Mehta, 1981; Dent et al., 1982, Kono et al., 1985; Kyriakides et al., 1986; Schihl et al., 1996) and more comprehensive multi-zone models (Hiroyasu et al., 1983; Lipkea and DeJoode, 1987; Kouremenos et al., 1986, 1987, 1997; Bazari, 1992; Li and Assanis, 1993; Mehta et al. 1995; Jung and Assanis, 2001).

In parallel to these mixing approaches a number of strictly empirical models were developed and are

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employed within various engine cycle simulation computer codes (Watson, 1977; Watson et al., 1980; Ghojel, 1982; Miyamota et al., 1985; Craddock and Hussain, 1986; Breuer, 1995; Reddy et al., 1996) such as Transeng, GT-Power and Wave. Such correlations include a number of constants (up to six) that are not always a direct function of the engine system, i.e. fuel injection event, piston design, thus making a priori optimized combustion system design nearly impossible. Nevertheless, such correlations are valuable for establishing an initial engine system configuration and thus save precious time throughout the development process. The engine community also saw development of three-dimensional models during this same time period that are currently employed for fine tuning combustion system geometry and targeting with codes such as KIVA (Amsden et al., 1985, 1989).

The LSCM is also a bulk mixing approach but includes relevant combustion chamber design parameters (spray impingement length, mean bowl wall curvature, bumper clearance, etc.) and the injection event (fuel velocity, number of nozzle holes and size, and angle) qualifiers on the heat release event through judicious selection of three constants – spray angle, laminar flame speed, and viscous dissipation (Schihl et al., 1999, 2002). The first constant is the most difficult to assess and usually is chosen based on measurements acquired by various researchers in engines and in combustion bombs; the second constant is actually a physicochemical property of the fuel; the last constant represents the turbulent dissipation rate and tends to be on the order of a tenth based on a number of engines modeled in the past. Overall, the elimination of laminar flame speed as a constant would reduce LSCM down to a single constant model assuming that the dissipation rate is on the same order for a given combustion chamber geometry (Schihl and Tasdemir, 2004).

Experimental determination of laminar flame speed for heavy hydrocarbon fuels is difficult. Most measurements reported to date range in fuel type from hydrogen to octane over a variety of temperatures, pressures, and air-fuel ratios (Andrews and Bradley, 1972; Metghalchi and Keck, 1982; Law, 1993; Zhou and Garner, 1996; Kobayashi et al., 1996; Egolfopoulos et al., 1998; Daly et al., 2001; Hirasawa et al., 2001). Two recent attempts to directly measure laminar flame speed for diesel fuel and jet fuel (JP-8) were unsuccessful due to the associated fast pre-ignition chemistry (personal communications with Southwest Research Institute and Northeastern University). Given the experimental limitations of obtaining this key combustion parameter, an indirect method was developed to assess diesel fuel laminar flame speed behavior as a function of ignition temperature and pressure based on heat release data acquired from two diesel engines. The underlying assumption of this method is that the spray mixing layer fuel consumption rate can be determined if the turbulent intensity is known and the flame sheet is thin in comparison to the mean eddy length scale (Turns, 1996). Based on experience with various engines it should be possible to properly scale turbulence intensity given the good agreement between LSCM predictions and heat release data over various engine speed-load conditions (Schihl et al., 1999, Schihl et al., 2002). Additionally, utilization of a large database of engine operating conditions will also minimize any experimental and modeling errors associated with indirect determination of the associated heat release profiles.

1. EXPERIMENTAL SETUP

Two direct injection diesel engines were employed for this study as shown in table 1. The smaller bore engine was a single cylinder automotive-type (Schihl et al., 2002) while the larger bore engine was a two cylinder engine variant of the Bradley Fighting Vehicle V-8 power plant (Schihl et al., 2001). Each engine was operated over a variety of speed and load conditions, and included piezo-electric transducers for measuring combustion chamber pressure for heat release analysis. Additionally, the smaller bore engine was also operated at various exhaust recirculation (EGR) levels, fuel injection pressures, and injection timing schedules.

TABLE 1: ENGINE SPECIFICATIONS

Engine Parameter	Description	
Model Type	Cummins V903	Ford DIATA
Number of Cylinders	2	1
Injection system	PT	FEV CORA II
Injection pressure[1] (bar)	600 – 1300	500 –1200
Nozzle geometry (mm)	7 x 0.190	6 x 0.124
Bore x stroke (mm)	140 x 125	70 x 78
Compression ratio	12.5	19.5
Swirl number	0.8	2.4[2]
Displacement[3] (cc)	1850	300
Operating speeds (rpm)	1600 – 2600	1500 – 3000
IMEP range (bar)	5 – 14	3 – 18
Boost system	Shop air	

1 Peak value.
2 Flow bench demonstration at maximum valve lift.
3 Per cylinder.

Heat release analysis was performed using standard thermodynamic first law analysis and the perfect gas law. The specific heat ratio was calculated based on an ideal gas mixture of CO_2, H_2O, N_2, O_2 and gaseous diesel fuel when appropriate, i.e. after start of injection, and the bulk cylinder temperature was determined based on corrected real gas behavior (Kanimoto et al., 1997) and estimated in-cylinder charge mass – the corresponding equation of state is given by:

$$\nu = \frac{RT}{P} + 1.09059\,x\,10^{-3} - \frac{8.50053x10^{-3}}{(T/100)^{1.64}} + \frac{4.34248x10^{-10}}{(T/100)^{2.49}}P - \frac{6.52579x10^{-18}}{(T/100)^{2.92}}P^2 + \frac{2.95689x10^{-26}}{(T/100)^{3.17}}P^3 \quad (1)$$

The initial specie mole fractions were chosen (CO_2, H_2O, N_2, O_2) after the intake valve closing event and a single step global paraffin chemistry model was utilized to determine any changes in the specie mole fractions upon initiation of the injection process. Since the apparent heat release rate does not differentiate between heat transfer and gross burning rate, and typical combustion efficiencies in diesel engines are 99%, a speed up factor was incorporated within the chemistry model to ensure a nearly complete burn and thus a more accurate calculation of the charge specific heat ratio. All experimental pressure traces were conditioned with a digital low pass filter that had a cutoff frequency of typically twice the engine speed preceding heat release analysis and n-hexadecane was chosen as a surrogate fuel for DF-2 based on a previous heat release fuel sensitivity study (Schihl et al., 2002).

1.1 Fuel Effects

A commercial DF-2 was employed throughout evaluation of the Ford DIATA engine while a military grade DF-2 was utilized throughout the V903 test schedule. Details of each fuel are given in table 2.

TABLE 2: TEST FUEL SPECIFICATIONS

Fuel Parameter	Engine Configuration	
	Cummins V903	Ford DIATA
Density (kg/m^3)	845	842
Cetane Number	47	53
Net Heating Value (MJ/kg)	42.6	42.8
Hydrogen (% wt.)	12.8	13.25
Sulfur (ppm)	1400	400

2. PREMIXED PHASE COMBUSTION MODEL

The combustion event maybe idealized as a sequence of three major events as described in the past by LSCM – ignition, consumption of the fuel-air mixing layer, and consumption of mixing controlled fuel-air packets (Schihl et al., 1999). During the ignition delay period, a mixing layer forms on the fuel spray periphery comprised of varying local fuel-air ratios and temperatures that is highly dependent of the fuel jet injection profile and in-cylinder thermodynamic state. At some point, a packet or packets of fuel-air charge reach an excited state that results in stabilization of a flame kernel and thus the onset of ignition once exothermic energy release exceeds the local diffusion/convection transport rates. Afterward, the flame front(s) propagate in rapid fashion throughout the mixing layer consuming packets that reach flammable limits at a rate the order of the fuel injection velocity (Balles and Heywood, 1989). This consumption process is commonly referred to as the premixed phase of combustion (Heywood, 1988). After ignition, other fuel packets not originally included within the mixing layer either begin or continue to mix locally with oxidizer. Eventually these packets reach proper proportions and are eventually consumed by the established frame front initiated during the premixed phase of combustion. The mixing controlled phase of combustion initiates upon consumption of these packets and is assumed to occur at stoichiometry as is typical of a diffusion flame.

The LSCM addresses each of the three events based on simplified physics and inherently includes a premixed phase submodel that is based on the flamelet assumption (Turns, 1996) originally employed in homogeneous charge spark-ignition engines (Blizzard and Keck, 1974; Tabaczynski et al., 1977) and modified for diesel sprays (Schihl et al., 1999) as given below:

$$\frac{dm_{en}}{dt} = FA\rho\ A_f\ (\tilde{u} + S_l + U_{jet})$$
$$\frac{dm_{pb}}{dt} = \frac{m_{en} - m_{pb}}{\tau} \quad (2)$$
$$\tau = \frac{\delta_t}{S_l} \qquad \frac{\delta_t}{l} \propto \mathrm{Re}_l^{-0.5} \qquad \mathrm{Re}_l = \frac{\rho \tilde{u} l}{\mu}$$

where m_{en} is the mixing layer charge mass entrainment rate, FA is the average mixing layer fuel-air ratio, ρ is the charge density, A_f is the flame front area, $\tilde{u}$ is the mean turbulence intensity, S_l is the laminar flame speed, U_{jet} is the local jet penetration rate, m_{pb} is the consumed premixed phase fuel mass, τ is the characteristic burning time, δ_t is the Taylor length scale, l is the representative mixing length scale and μ is the charge viscosity. Furthermore, the flame front area and mean turbulence intensity is given below:

$$\tilde{u} = l\,\omega \qquad A_f = \pi\left[(R' + \delta_{pm})^2 - R'^2\right] \quad (3)$$

and ω is the bulk mixing rate, R' is the radial distance from the spray centerline to the onset of the shear layer, and δ_{pm} is the premixed fuel-air shear layer thickness (Dimotakis, 1991). The representative eddy length scale is chosen as the following inverse relationship:

$$\frac{1}{l} = \frac{1}{B} + \frac{1}{z + d} \quad (4)$$

and B is the cylinder bore, d is a representative bowl depth, and z is the distance from the piston lip to the fire deck. The bulk mixing rate is determined based on

contributions from the injection event, squish flow, swirl, dissipation, and combustion chamber compression-expansion. Fundamentally it is derived from the angular momentum of a representative eddy (Spalding, 1970) as shown below:

$$\begin{aligned} \frac{d\Omega}{dt} &= \dot{P}_{inj} + \dot{P}_s + \dot{P}_{sw} - \dot{D}_s \qquad \Omega = \frac{1}{8} m_e \omega l^2 \\ \frac{dm_e}{dt} &= \dot{m}_{inj} + \dot{m}_{sq} \qquad \dot{P}_s = ABS(\dot{m}_{sq} U_{sq} l_{sq}) \\ \dot{D}_s &= a\omega\Omega \exp(-a\omega\delta t) \qquad \dot{P}_{inj} = \frac{\dot{m}_{inj} U_{inj} S}{4} \\ \dot{P}_{sw} &= \rho\left(\frac{S+L_b}{2}\right)^3 \omega_s^2 \left\{\tan\left(\frac{\theta}{2}\right)\right\}^2 \frac{S^2 - L_b^2}{2} \end{aligned} \quad \textbf{(5)}$$

where $\dot{P}_{inj}$ is the injection production term, $\dot{P}_s$ is the squish production term, $\dot{D}_s$ is the dissipation term, m_e is the eddy mass, $\dot{P}_{sw}$ is the swirl production term, $\dot{m}_{inj}$ is the injection rate, $\dot{m}_{sq}$ is the squish mass flow rate, U_{sq} is the average squish velocity, l_{sq} is the squish length scale, a is the dissipation constant, U_{inj} is the injection velocity, δt is the calculation time step, L_b is the break-up length, θ is the spray cone angle, ω_s is the swirl rate, and S is the spray tip penetration distance. The squish mass flow rate is determined based on piston speed, squish area, and bulk density (Heywood, 1998) and the squish length is defined as – (z/2 + l/4).

Last, the spray formation process is a two zone model (Hiroyasu and Arai, 1980) that is applicable both to the liquid dominated and gaseous regimes. For completeness, this model is given below:

$$\begin{aligned} t < t_b \qquad & S(t) = B\, U_{inj}\, t \qquad t_b = \frac{\alpha \rho_l d_o}{(2c_1 \rho \Delta P)^{0.5}} \\ t > t_b \qquad & S(t) = \frac{2.95}{B^*} \left(\frac{\Delta P}{\rho}\right)^{0.25} (d_o\, t)^{0.5} \end{aligned} \quad \textbf{(6)}$$

where B and B* are constants, t_b is the break-up time, d_o is the orifice diameter, α and c_1 are break-up constants, ΔP is the orifice pressure drop, and ρ_l is the injected fuel density.

The three major parameters controlling the premixed phase burn rate are the laminar flame speed, spray angle, i.e. flame front area, and the turbulence intensity. The former is a function of the fuel and thermodynamic state of the mixture and fundamentally is described below:

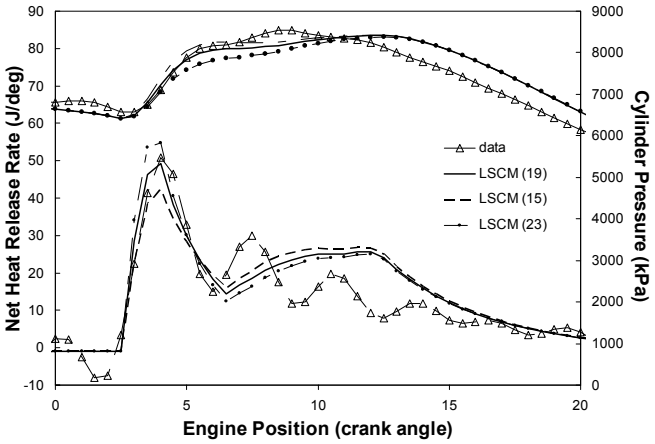

Figure 1: LSCM Laminar Flame Speed Calibration at Light Load for DIATA Engine.

$$S_l = S_{l,o} \left(\frac{T}{T_o}\right)^2 \left(\frac{P}{P_o}\right)^a \left(\frac{O_2}{O_{2,o}}\right)^b \quad \textbf{(7)}$$

where o-subscripted parameters represent reference conditions, T is the mean cylinder temperature at ignition, P is the cylinder pressure at ignition, O_2 is the oxygen concentration, and a and b are fuel dependent constants. These latter constants are ideally determined through a best fit of experimental data but that option is currently not available for DF-2 as discussed within the introduction.

Last, the LSCM mixing controlled phase is a characteristic time model that has been extensively discussed in the past (Schihl et al., 1999; Schihl et al., 2002). Essentially, the mixing time is the conjugation of four time scales – the bulk mixing time, the wall effect, an EGR based oxygen displacement, and an air utilization correction that collectively dictate both the mixing and fuel consumption rates. As noted earlier, the consumption rate is controlled by the turbulence intensity.

3. RESULTS

LSCM was optimized to match experimental in-cylinder pressure traces and corresponding heat release profiles through selection of the optimal laminar flame speed over various engine operating conditions. One key assumption made throughout this process involved the judicious selection of the jet formation angle. The methodology for this study entailed referencing various published spray angle data literature and scaling such measurements based on charge density and nozzle geometry to match each engine and associated operating condition (Su et al., 1995; Hiroyasu and Arai, 1990; Ruiz and Chigier, 1991; Montgomery et al., 1996; von Kuensberg Sarre et al., 1999; Han et al., 2000; Bae and Kang, 2000).

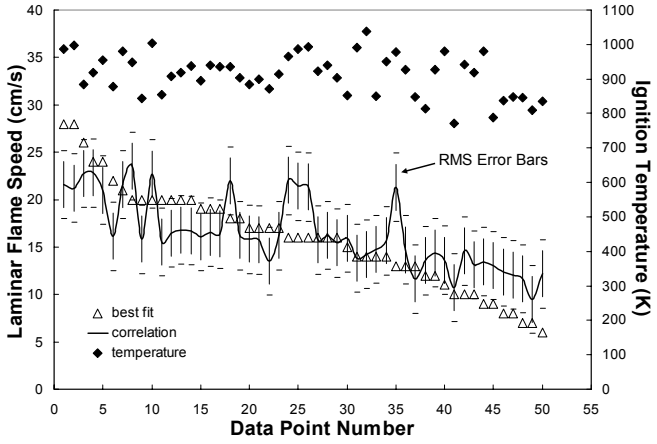

Figure 2: Comparison of Laminar Flame Speed Correlation with LSCM Best Fit Values.

An example of this optimization process is demonstrated by figure 1. The choice of the larger laminar speed value (23 cm/s) resulted in an over prediction of the peak premixed phase burning rate while choice of the lower laminar flame speed (15 cm/s) has the converse effect. For this particular case, the choice of the optimal laminar flame speed (19 cm/s) matched both the heat release and cylinder pressure profiles in an acceptable manner that implies LSCM did properly capture the mixing time scales. A total of seventy-seven operating points were subjected to this optimization method, but only fifty were accepted and included in this study since twenty-seven of the points did not exhibit a precise enough agreement with the experimental profiles.

Furthermore, the laminar flame speed correlation is a function of charge pressure, temperature, and equivalence ratio. These latter two parameters vary with time during the post-ignition flame spread event since the mixing layer is stratified in both composition and reactant temperature. In order to simplify this complex event, the bulk temperature and pressure, and oxygen concentration at the spray tip at ignition were chosen as representative values throughout the premixed phase of combustion. Additionally, the spray tip oxygen concentration at ignition was determined based on penetration distance at ignition (Schihl et al., 2002).

The two test fuels employed in this study had similar bulk properties as shown in table 2 but had varying cetane number and sulfur concentration levels. This study made the assumption that the reference laminar flame speed did not vary drastically between the two fuel samples and that bulk composition was similar enough to ensure each fuel demonstrated approximately the same trend versus cylinder temperature, pressure, and spray tip mean air-fuel ratio (Schihl et al., 2004).

The overall behavior of the optimal (best-fit) laminar flame speed and the associated correlation is given in

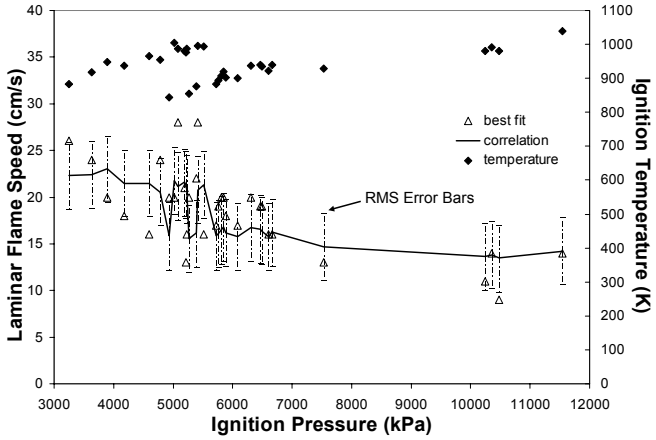

Figure 3: Comparison of the Laminar Flame Speed Correlation with the LSCM Best Fit Values for Non-EGR Operating Conditions.

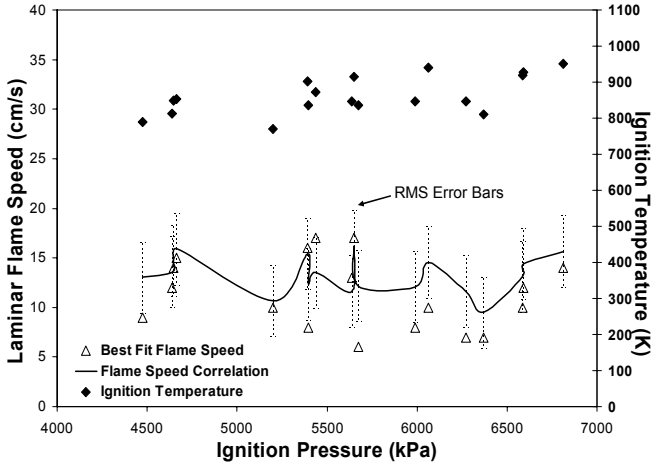

Figure 4: Comparison of the Laminar Flame Speed Correlation with the LSCM Best Fit Values for EGR Operating Conditions.

figure 2. Data is presented in a monotonically decreasing order versus measured cylinder ignition pressure in order to study thermodynamic trends in laminar flame speed since the overall behavior is complex. Inherent in this data set are eighteen EGR points that were acquired from the Ford DIATA. Note that the best-fit laminar flame speed varied between 6 cm/s and 30 cm/s with an associated bulk ignition temperature ranging from 800 K to 1040 K as dependent on the speed-load operating point. Additionally, the spray tip oxygen mass fraction was much less at the lower range of the best-fit flame speed spectrum in part due to EGR that varied between 10% to 45% and the associated lower ignition temperatures versus non-EGR cases. This later observation is apparent by studying the non-EGR and EGR cases as given in figures 3 and 4. Last, cool flame operating conditions were excluded from this study since LSCM does not address low temperature chemistry heat release (Schihl et al., 1999).

The resulting laminar flame speed correlation exhibited a root-mean-square (RMS) error of ±3.6 cm/s in comparison to the best-fit values. Overall only a small portion (six) of the best-fit values fell well outside the RMS error but this shortcoming is not that significant considering a zero-dimensional combustion model was employed in this study. The implication is that LSCM generally captured the bulk mixing profile to sufficiently predict the net heat release profiles in two distinctly different direct-injection diesel engines over a variety of operating conditions. The resulting correlation is given below:

$$S_l = 21\left(\frac{T}{300}\right)^2 P^{-0.6}\left(\frac{Y_{O_2}}{0.21}\right)^{0.3} \quad \textbf{(8)}$$

where S_l has units of cm/s, P and T have units of bar and Kelvin, and Y_{o2} is the spray tip oxygen mass fraction.

CONCLUSION

A method to indirectly determine the laminar flame speed was developed for direct injection diesels based on using a zero-dimensional two-phase combustion model to match experimental pressure and heat release profiles. Data acquired for both light-duty and heavy-duty engines was employed in this study and revealed a laminar flame speed correlation that had realistic trends and magnitude in comparison to lighter hydrocarbon fuels. The correlation is limited to non-cool flame operating conditions since the zero-dimensional combustion model employed in this study did not include low temperature chemistry capability. This correlation maybe employed in three-dimensional flame models used for diesel applications and thus could be used for future military high output engine development efforts.

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