Full Length Article

Burning velocity and Markstein length blending laws for methane/air and hydrogen/air blends

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ABSTRACT

Because of the contrasting chemical kinetics of methane and hydrogen combustion, the development of blending laws for laminar burning velocity, u_l, and Markstein length for constituent mixtures of CH_4/air and H_2/air presents a formidable challenge. Guidance is sought through a study of analytical expressions for laminar burning velocity. For the prediction of burning velocities of blends, six blending laws were scrutinised. The predictions were compared with the measured burning velocities made by Hu et al. under atmospheric conditions [1]. These covered equivalence ratios ranging from 0.6 to 1.3, and the full fuel range for H_2 addition to CH_4. This enabled assessments to be made of the predictive accuracy of the six laws. The most successful law is one developed in the course of the present study, involving the mass fraction weighting of the product of u_l, density, heat of reaction and specific heat, divided by the thermal conductivity of the mixture. There was less success from attempts to obtain a comparably successful blending law for the flame speed Markstein length, L_b, despite scrutiny of several possibilities. Details are given of two possible approaches, one based on the fractional mole concentration of the deficient reactant. A satisfactory empirical law employs mass fraction weighting of the product $u_l L_b$.

1. Introduction

There is increasing interest in supplementing natural gas supplies with the addition of hydrogen. This has led to a number of experimental and chemical kinetic [1,2] studies of the burning velocities, u_l, of such blends with air. The interest in this extends beyond such practicalities to the general problem of deriving satisfactory blending laws for fuel/air mixtures, with very different burning velocities and chemical kinetics. For example, the laminar burning velocity, u_l, of a stoichiometric mixture at 303 K and 0.1 MPa of CH_4 is 0.35 m/s, whereas that for H_2/air is 2.05 m/s. This large difference makes the prediction of CH_4/H_2 burning velocities a particularly challenging test for blending laws.

One of the approaches adopted is based on earlier analytical derivations of expressions for the laminar burning velocity, involving profiles of volumetric heat release rates. An important difference in flame structure between CH_4/air and H_2/air flames is revealed by the profiles of the volumetric heat release rates, normalised by their maximum values, q/q_{max}, and plotted against the reaction progress variable, c. Values of such profiles computed from earlier detailed chemical kinetics studies [3] are shown in

Fig. 1 by the two contrasting dotted curves. The full line curve is a more approximate algebraic fit. The maximum heat release rate of the faster burning H_2 mixture occurs at a distinctively lower value of c. This is a consequence of enhanced molecular transport and low temperature reaction, both attributable to H atoms, with a resulting increase in u_l. The kinetic modeling in [2] shows how the blend u_l of CH_4/H_2 flames increases with the concentration of H. Exceptionally, in hydrogen flames, such is the upstream diffusion of H atoms and the consequent induced reactivity, the concept of a flame thickness based on an inert preheat zone is of limited validity [4]. The contrasting aspects of CH_4 and H_2 flame structures make the development of accurate blending laws for u_l values of their blends more exacting than the development of such laws for hydrocarbon blends.

The present paper explores the application of six different laws, for predicting the burning velocities of blends of CH_4/air and H_2/air, at the same equivalence ratio, ϕ. One of the laws is entirely new and was developed in the course of the present study. Probably the earliest blending law was that of Le Châtelier [5] for predicting the lean flammability limit of a blend, based upon the reciprocal of mole fraction weighting of those of the constituent fuels. A common approach is to employ a property of the constituent mixtures, all at the same ϕ, designated by i and j for a binary blend, with an appropriate quantitative weighting of that property. Frequently

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Nomenclature

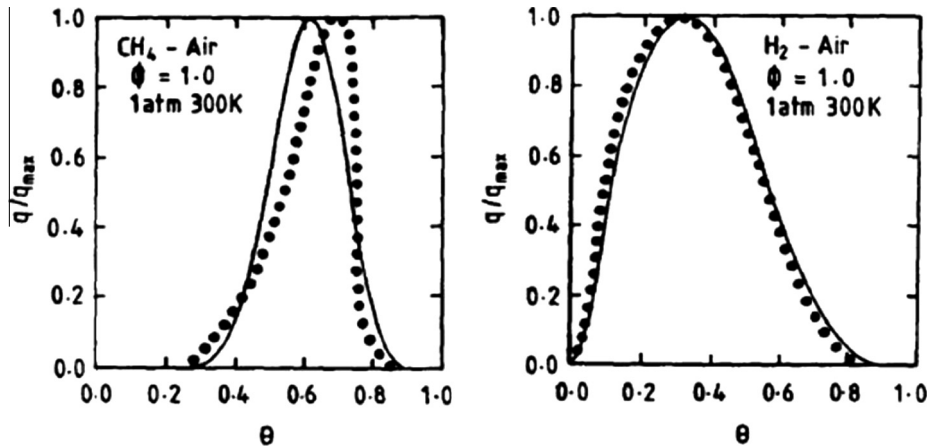|				
a	air mole/fuel mole		T_{al}	activation temperature, based on $u_l\rho_u$ (K)
a_s	stoichiometric air mole/fuel mole		$\widetilde{T}_a$	activation temperature based on u_l (K)
c	reaction progress variable		T_u	unburned temperature (K)
c_p	mean specific heat at constant pressure (J/mass/K)		T_b	burned temperature (K)
h	sensible enthalpy (J/mol)		u_l	unstretched laminar burning velocity (m/s)
h_f	enthalpy of formation (J/mol)		$\bar{x}$	mixture mole fraction
k_u	mixture thermal conductivity (J/m/K/s)		$\bar{x}_f$	fuel mole fraction
k_m	mean thermal conductivity (J/m/K/s)		$\bar{x}_i$	i'th constituent mole fraction
L_b	burned gas Markstein length (m)		x	mass fraction
Le	Lewis number		x_f	fuel mass fraction
Ma_b	burned gas Markstein number		x_i	i'th constituent mass fraction
$\bar{m}_i$	species i mole fraction		$\bar{x}_d$	deficient reactant mole fraction
$\bar{m}_R$	reactant mole fraction		Z	Zel'dovich number $= \left(T_a/T_b^2\right)(T_b - T_u)$
P	pressure (Pa)			
q	heat release rate (J/s)		*Greek symbols*	
q_{max}	maximum volumetric heat release rate (J/m^3 s)		α	flame stretch rate (1/s)
$\overline{Q}$	molar heat of reaction (J/mol)		δ	flame thickness (m)
Q	mass heat of reaction (J/kg)		λ	burning velocity eigenvalue
$R(c)$	heat release rate source term (J/m^3 s)		υ	kinematic viscosity (m^2/s)
r	laminar flame radius (m)		ρ_u	unburned mixture density (kg/m^3)
S_n	stretched flame speed (m/s)		ρ_b	burned mixture density (kg/m^3)
S_s	unstretched flame speed (m/s)		ϕ	equivalence ratio
t	time (s)			
T	temperature (K)			

Fig. 1. Dotted curves show volumetric heat release rate profiles from detailed chemical kinetics, for CH$_4$/air and H$_2$/air mixtures from [3]. θ is the reaction progress variable, *c*. The full line curve is a more approximate algebraic fit.

the property employed is the laminar burning velocity of the constituent mixtures, u_{li}, along with mole or mass fractional weightings, $\bar{x}_i$, or, x_i, respectively, of the constituent mixtures. The burning velocity of the blend, u_{lb}, expressed in terms of the fractional mass concentrations of the constituent fuel/air mixtures, x_i and x_j and their respective burning velocities is:

$$u_{lb} = x_i u_{li} + x_j u_{lj}. \tag{1}$$

The expression for fractional mole weighting, indicated by $\bar{x}_i$ is similar.

Burning velocities also are affected by the flame stretch rate and, for this, a convenient and relevant parameter is the Markstein length, L_b. This can be derived directly from flame speed measurements in spherical explosions, as in [1]. The chemical kinetic computational studies in [6] show how Markstein lengths can be

derived from these, that are associated, with the laminar burning velocity and the separate effects of both strain rate and flame curvature. This is applied to experimentally measured values in [7]. Normalised by the laminar flame thickness these give the corresponding Markstein numbers. In contrast to u_l, no blending laws are known to the authors for L_b.

Two possible approaches for Markstein length blending laws are considered. One is based on weighting the value of L_b for each constituent mixture by the fractional mole concentration of the deficient reactant (fuel or oxygen). The other, involves fractional mole concentration weighting of the product $u_l L_b$ for each constituent mixture.

The different blending laws for u_l and L_b are first formulated and discussed. Each is then employed to predict the values of these parameters for blends of CH$_4$/air and H$_2$/air at the same ϕ, over