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Formalism for spatially averaged consumption speed considering spherically expanding flame configuration

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ABSTRACT

The determination of laminar burning velocity is a complex task. Even though its definition is well established, achieving a good and reliable value of this quantity seems to be too dependent on the experimental procedures. In this study, we report a rigorous derivation of the relation between the spatially averaged consumption speed and the absolute flame speed for spherically expanding flame configurations. The general expression of the consumption speed in confined geometries makes it possible to retrieve classical definitions developed in the literature over the years. It has been highlighted that the analytical development for the consumption speed is free from restrictive assumptions or approximations (stretch or thermodynamical gas states) that are generally made in classical approaches. The development brings up to identify two equivalent radii, one from a surface and one from a volume integration, respectively. The analytical developments are tested using a 3D DNS including full transport and complex chemistry. CH_4/air flame at three equivalence ratios (lean, stoichiometric and rich) and a stoichiometric iso-octane/air flame are tested. Results show that any species, reactants or products, can be used to evaluate the analytical expression of the consumption speed.

1. Introduction

Recent advances in numerical simulations have demonstrated the ability of CFD codes to simulate and accurately predict complex combustion processes from fuel injection to pollutant emissions. It is worth noting that pollutant emission regulation is a key parameter in designing combustion systems such as aircraft engines, helicopter turbines or industrial burners. With the emergence of new fuels, the corresponding kinetic schemes need to be developed and validated for large ranges of operating conditions, expressed in terms of equivalence ratio, pressure and temperature. Kinetic schemes are generally validated based on ignition delays time, major and/or minor species profiles and unstretched laminar burning velocity S_l^0 data.

Laminar burning velocity S_l^0 is a fundamental flame property which depends on the fuel/air mixture and its initial thermodynamic conditions: pressure, temperature and equivalence ratio. It represents the rate at which the fresh gases are consumed through the flame front considering a 1D unstretched propagating planar premixed flame. By integrating the transport equation of fuel mass fraction over the flame domain, one can easily derive the expression of the laminar burning velocity for 1D planar flames [1] as:

$$S_l^0 = \frac{1}{\rho_u \left(Y_{f,b}^{th} - Y_{f,u}\right)} \int_{-\infty}^{+\infty} \dot{\omega}_f dx, \tag{1}$$

where ρ_u is the fresh gas density, $\dot{\omega}_f$ is the fuel reaction rate, and $Y_{f,u}$ and $Y_{f,b}^{th}$ are the fuel mass fractions in the fresh and burned gases, respectively.[1] The laminar burning velocity S_l^0 is a consumption speed and corresponds to the fuel mass rate which enters the flame front. It is worth noting that the expression of the laminar burning velocity is valid for any species k. For the 1D geometrical configuration, S_l^0 also corresponds to the flame displacement speed relative to the fresh gases, $S_{d,u}^0$. The latter represents the motion of the flame and is defined as the speed of an iso-surface relative to the flow of reactants [1–3] as:

$$S_{d,u}^0 = S_f - u_{g,u}, \tag{2}$$

where $u_{g,u}$ refers to as the fresh gas side velocity. S_f is the absolute flame speed or propagation speed. Since the flow accelerates

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[1] The upper script th denotes that the burned gases are taken at equilibrium conditions. In the following, the density ρ_b^{th} and the mass fraction of a specie k in burned gases $Y_{k,b}^{th}$ will be obtained from equilibrium code.

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Nomenclature

Acronyms

DS	deficient species
DWFDS	density weighted flame displacement speed
SEF	spherically expanding flame
Thin	infinitely thin flame

Greek symbols

$\dot{\omega}_k$	reaction rate of the k_{th} reaction
γ	heat capacity ratio
ϕ	equivalence ratio
κ	flame stretch rate
ρ	gas density

Subscripts and superscripts

0	flame properties considering the 1D unstretched planar flame configuration
b, u	referring to as burned and fresh sides, respectively
th	chemical equilibrium state

Roman symbols

$\mathbf{n}$	unit vector normal to the flame surface directed from the burned to the unburned side
P	pressure
S_f	absolute flame speed or propagation speed
ℓ_c	Markstein length
$\langle S_{c,i} \rangle$	spatially averagedflame consumption speed as defined
$\widetilde{S_{d,i}}$	density weighted flame displacement speed (DWFDS) as defined
I_0	stretch factor
R	flame radius
R_0	chamber internal radius
$R_{eq,k}$	equivalent flame radius associated to species k (Surface weighted integral)
$R_{eq2,k}$	equivalent flame radius associated to species k (Volume weighted integral)
R_{eq}	equivalent flame radius based on the total mass of deficient species
S_l^0	unstretched laminar burning velocity
$S_{d,i}$	flame displacement speed as defined
u_{g,r_i}	flow velocity as defined at $r = r_i$
Y_c	flame progress variable
$Y_{k,i}$	mass fraction of species k in state k

through the flame front due to gas expansion, the flame displacement speed (FDS), S_d^0, changes accordingly. Therefore, the FDS depends on the considered position chosen for its evaluation. It can be weighted by the ratio of the local density to the density of the reactants and is constant across the flame front. This density weighted flame displacement speed (DWFDS) is [3]:

$$\widetilde{S_d^0} = \frac{\rho}{\rho_u} S_d^0 = Cte. \tag{3}$$

However, when the flame is stretched (curved, strained, or both), all the flame displacement speeds are different and the flame response in terms of flame speed to flame stretch ratio may be significantly different. Recently, Giannakopoulos et al. [3] evaluated the influence of the iso-surface representing the flame surface for calculating the density weighted displacement speed for spherical/cylindrical expanding flames. By combining rigorous asymptotic development and 2D axisymmetric spherical simulations, Giannakopoulos et al. [3] showed a wide spread of slopes for DWFDS with flame stretch depending on the isotherm selected to represent the flame surface. Moreover the flame sensitivity to stretch may include a change of sign. For stretched spherical flames considering the fresh gas side, the DWFDS yields:

$$\widetilde{S_{d,u}} = \frac{dR}{dt} - u_{g,u}. \tag{4}$$

Subscript u refers to as the fresh gas side. $\frac{dR}{dt}$ is the absolute flame speed (or propagation speed S_f) obtained from the time derivative of the flame radius R evolution, which is easily measured experimentally either by shadowgraphy, Schlieren or laser tomography. The experimental determination of the relative displacement speed $\widetilde{S_{d,u}}$ is a complex task since it requires an accurate measurement of the fresh gas velocity at the entrance of the flame front. Recent developments of PIV post-processing have been performed by [4,5] in order to directly measure the local fresh gas velocity $u_{g,u}$. This value corresponds to the maximum value of the fresh gas velocity profile across the flame front. DNS studies demonstrated that this displacement speed relative to the fresh gases is insensitive to thermal radiation [6]. Therefore considering kinetic scheme validations, Eq. (4) remains a suitable expression for direct comparisons between experiments and a DNS of the experiments. Nevertheless, $\widetilde{S_{d,u}}$ is very sensitive to the value of the isotherm. A slight change in the isotherm drastically modifies the slope of the flame displacement speed and flame stretch correlation [3].

Considering the burned gas side, the DWFDS yields:

$$\widetilde{S_{d,b}} = \frac{\rho_b}{\rho_u}\left(\frac{dR}{dt} - u_{g,b}\right). \tag{5}$$

Subscript b refers to as the burned gas side. In this expression, ρ_b is generally assumed to be stationary and equal to the adiabatic value of burned gas density during the flame propagation. The burned gas velocity, $u_{g,b}$, is slightly negative when heat losses and/or compression effects are considered [7]. However, $u_{g,b}$ is null for adiabatic and unconfined expanding flames. Therefore, Eq. (6) is generally used in the literature, and in most of the cases, experiments report stretched propagation flame speed data as:

$$\widetilde{S_{d,b}} \simeq \frac{\rho_b^{th}}{\rho_u} \frac{dR}{dt}, \tag{6}$$

where ρ_b^{th} is the burned gas density at adiabatic thermodynamical and chemical equilibrium conditions. Recent theoretical and numerical works demonstrated that the proper isotherm for the evaluation of the DWFDS must be chosen sufficiently close to the burned gas side in order to get an ”unambiguous” behavior in the flame speed with stretch rate response [3]. However, the burned gas density of the stretched flame can be significantly different from the burned gas density at equilibrium conditions. Indeed, it was shown by [8] that the burned gas temperature of stretched flame was related to flame stretch and Lewis number. Preferential diffusion may over or under-estimate the stretched flame speed according to the Lewis number value. Consequently, this bias or difference between what we report and what we would like to measure leads to an additional uncertainty along the extrapolation process to get the laminar burning velocity. Moreover, both an inward flow induced by the density change in the burned gas [6] and heat losses [7] may affect the measured data. Also, it is worth noting that assuming an infinitely thin flame front, Eq. (6) should match the spatially averaged flame consumption speed [1, p. 83, Eq. (2.122)]:

$$\langle S_c \rangle_{Thin} \simeq \frac{\rho_b^{th}}{\rho_u} \frac{dR}{dt}. \tag{7}$$

A more precise formalism for the flame consumption speed must be derived with a minimal set of assumptions and should take into account the evolution of fuel mass fraction profile within the flame front thickness. Even though this contribution is expected to be small, it will affect the flame response to the flame stretch