Faculty of Engineering

Lean Premixed Turbulent Flames vs. Hydrogen Explosion: A Short Survey on Experimental, Theoretical and Analytical Studies

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Contents

Motivation:
Safety considerations in hydrogen usage in general and combustion in industrial applications

Study:
Restricted to deflagration flames, with the emphasis on molecular effects (preferential diffusion and Lewis number) on lean premixed turbulent combustion: Pure Hydrogen flames and Hydrogen-Hydrocarbon flames

Introduction

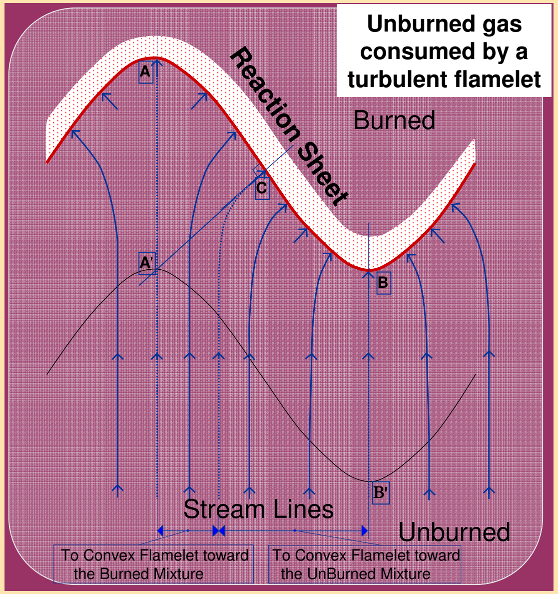
Experimental & theoretical convergence on lean hydrogen premixed turbulent flames (spherical explosions)

- Backward-facing flame fronts are formed nearer the unburned than the burned side of the turbulent flame brush, suggesting the importance of large-scale flame-front bulges in turbulent flame propagation
- Superadiabaticy and flame-front bulges convex toward the reactants are clearly observed, representing effects of the less-than-unity Lewis number of the mixture. The average size of flame bulges is found to increase with the turbulence integral length scale

(Karpov,) Lipatnikov and Chomiak, Proc. Combust. Sym. Int. 1996, & Prog. in En. and Combust. Sci 2005

Chen and Bilger, Combust. and Flame 2004

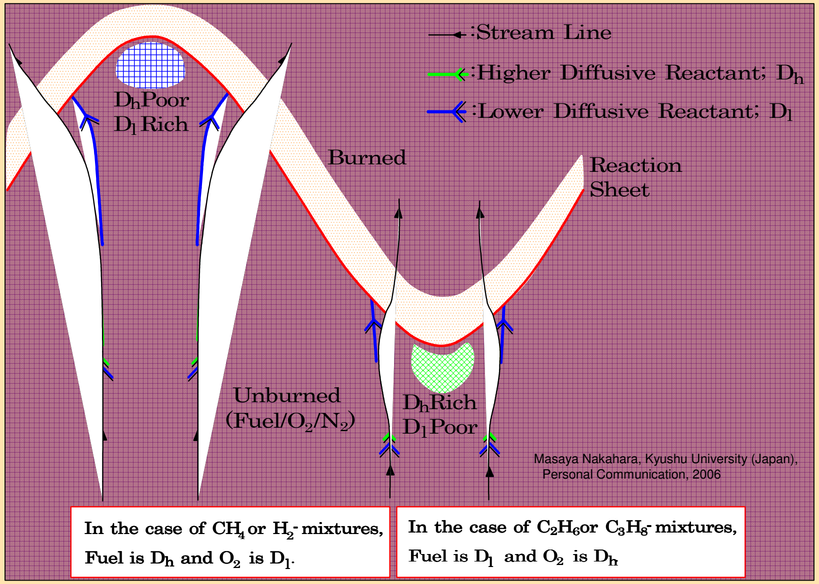
Flame Curvature, Mass Flow & Turbulent Flame Speed



1. Premixed gas flows along marked streamlines
2. Streamlines ⊥ to flamefront
3. Ratio of mass flow flowing into the convex 'BC unburned' / to convex 'AC burned' ~ 3:1
4. The convex part of flamelet towards the unburned mix. affects the turbulent flame speed predominantly

Masaya Nakahara, Kyushu University (Japan), Personal Communication, 2006

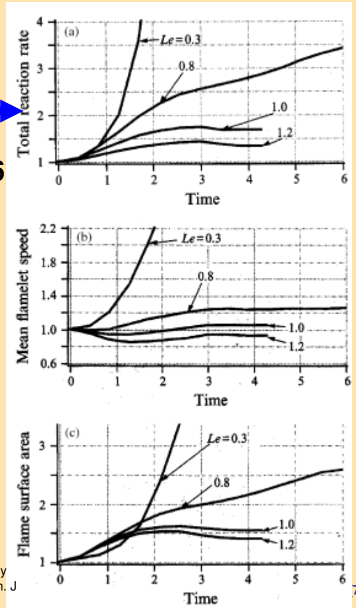
Preferential Diffusion and Lewis number Effects



Lewis Number Effects – DNS investigations

❖ DNS by Trouvé and Poinsot 1994 on lean $H_2/O_2/N_2$ flames………………………………………………………………………………… and DNS of lean H_2 flame by Bell et al. 2006 (not depicted here), confirm the Le influence on turbulent flame speed, especially in lean H_2 mixtures

❖ This substantial rise in flame speed may be due to sum of DL and PDT effects, or, can also be explained using Leading Point concept

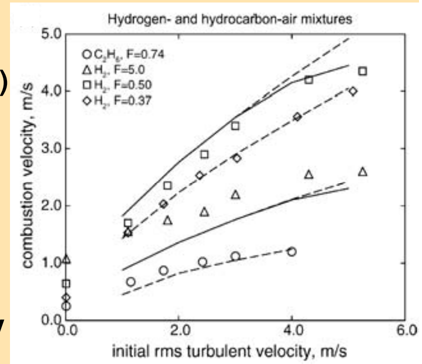


Trouve´ A, Poinsot T. Evolution equation for flame surface density in turbulent premixed combustion. J Fluid Mech 1994;278:1–31.

Lewis Number Effects – Russian database

❖ Case1: For lean (ϕ=0.5, Le =0.45) H_2 mixture, S_{L0} is 5 times lower as compared with a rich (ϕ=2.0, Le=1.9) H_2-air mixture, whereas the slope (S_T/u') shows the opposite behaviour and S_T is markedly higher for the former mixture at u'>1 m/s

❖ Case2: For very lean (ϕ=0.17, Le=0.4) H_2 mixture (not depicted here), S_{L0} is by more than 15 times lower as compared with the above rich case, while S_T for both cases are roughly equal



Karpov and Severin 1980, extracted from A.N. Lipatnikov, J. Chomiak / Progress in Energy and Combustion Science 31 (2005) 1–73

Premixed Turbulent Combustion Model

Algebraic flame surface wrinkling premixed turbulent reaction submodel by Muppala, Aluri and Dinkelacker

$$\frac{A_T}{\bar{A}} \approx \frac{S_T}{S_{L0}} = 1 + \frac{0.46}{Le} \mathrm{Re}_t^{0.25} \left(\frac{u'}{s_L}\right)^{0.3} \left(\frac{p}{p_0}\right)^{0.2}$$

$\frac{A_T}{A_L}$ = Normalized turbulent flame surface area

$\frac{S_T}{S_L}$ = Normalized turbulent flame speed

$\frac{u'}{S_L}$ = Turbulence-chemistry interaction

a = single pre-constant Le = Lewis number

Re_t = Turbulent Reynolds number p = Operating pressure

Ill to Bradley's relation

$$\frac{S_T}{S_{L0}} = 1 + \frac{0.95}{Le} \left(\frac{u'}{s_{L0}} \frac{l_x}{\delta_{L0}}\right)^{0.5}$$

Muppala et al. Combust. and Flame 2005, & Prog. in CFD 2004

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2. Premixed Turbulent Combustion Model

Above relation failed to demonstrate the influence of hydrogen on hydrocarbons, and moreover, for very lean pure hydrogen flames

Modifications were carried out on algebraic flame surface wrinkling premixed turbulent reaction submodel using the concept of Leading point related to critically curved flamelets

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Leading Point Concept -- Critically Curved Flamelets

- **To predict the strong effect of Lewis number on turbulent flame speed, critically curved laminar flames have been proposed as a model of the leading kernel structure by arguing that:**
  (1) the leading points should be associated with the highest local burning rate, and
  (2) highest (for various possible perturbations of a laminar flame with Le<1) local burning rate is reached in such flames. The latter hypothesis has been substantiated by simulations of various perturbed laminar flames.

- **Also, strongly curved, lean H_2–air flames can survive under the influence of high strain rates. This behaviour is associated with the local increase in temperature in curved laminar flames, because the energy flux into the flame exceeds the heat losses from it if Le<1.**

Lipatnikov and Chomiak, Combust. Sci. and Tech. 1998

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Leading Point Concept -- Critically Curved Flamelets

For Lewis numbers < 1, the flame ball temperature is given by

$$T_r = T_u + (T_b - T_u)/Le$$

The chemical time scale for the highest local burning rate is

$$\tau_{cr} = \tau_c \frac{R_{cr}}{\delta_{L0}} = \tau_c Le^{-1} \left(\frac{T_b}{T_r}\right)^{1.5} \exp\left(\frac{\Theta}{2T_b} \frac{T_b - T_r}{T_r}\right) \rightarrow \tau_{cr} = \tau_{c0} \frac{(u_c)_{t\to\infty}}{\max\{u_c(t)\}_{r=r_{cr}}}$$

$$S_T = S_{L0}\left(1 + \frac{0.46}{\exp(Le-1)} u'^{0.8} s_{Lo}^{0.2} \left(\frac{\tau_t}{\tau_{c0}}\right)^{0.25} \left(\frac{p}{p_0}\right)^{0.2}\right)$$

Modified AFSW reaction model

$$\tau_{c0} = \alpha / S_{L0}$$

The mass flux of the deficient reactant throu' the surface of the flame ball scales as R_{cr}^{-1}

Critical chemical time scale = chemical time scale x consumption rate (of undisturbed planar laminar flame)/maximum possible local consumption rate

(percepted at the convex part (positive curvature) of the flamelet facing towards unburned gas)

Aluri, **Muppala**, Dinkelacker Combust. and Flame 2006

Lipatnikov and Chomiak, Combust. Sci. and Tech. 1998

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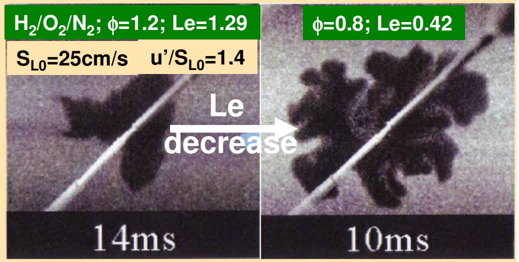
Expanding Spherical Turbulent Flames – Kido database

Hydrogen (40 flames)

ϕ = 0.5 to 0.95

Measured data:
S_L/S_{L0} = 1.0 to 3.1
mean local burning velocity / unstretched lami. fl. speed

$S_L = f(PD=D_f/D_o)$



Spherical gaseous (H_2) explosion

Nakahara, Kyushu University, Personal communication 2006

Model predictions

{without *PD* effect}

$$S_T = S_{L0}\left(1+\frac{0.46}{\exp(Le-1)}\mathrm{Re}_t^{0.25}\left(\frac{u'}{s_{L0}}\right)^{0.3}\right)$$

{without *Le (DT)* effect}

$$S_T = S_L\left(1+0.46\,\mathrm{Re}_t^{0.25}\left(\frac{u'}{s_L}\right)^{0.3}\right)$$

Correlation Plots for Hydrogen Flames – Kido database

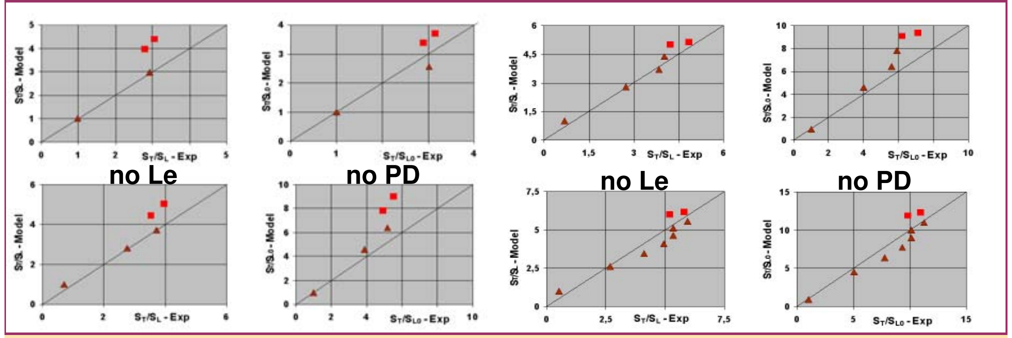
Left column –
$(S_T/S_L)_{Exp}$ vs. $(S_T/S_L)_{Model}$

S_L – mean local burning velocity

Right column –
$(S_T/S_{L0})_{Exp}$ vs. $(S_T/S_{L0})_{Model}$

S_{L0} – unstretched lam. fl. speed

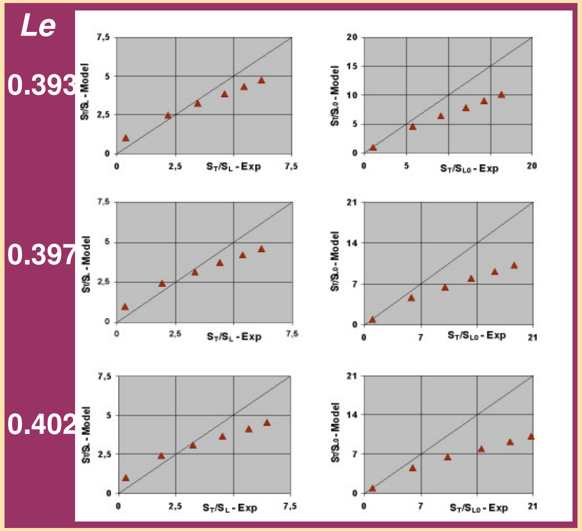
Le: 0.393 0.397 0.402 0.411



Correlation Plots for Hydrogen Flames – Kido database

S_L/S_{L0} = 2.7, 3.1, 3.3

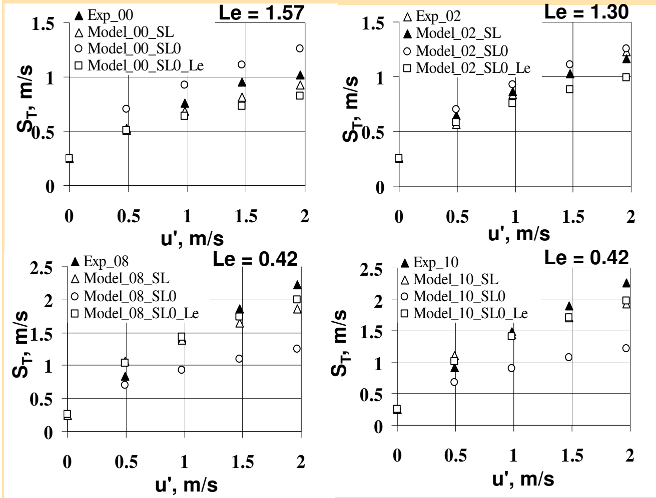
- Higher the ratio, greater the influence of PD
- The model predictions (RHS) deviate more for increased ratios.



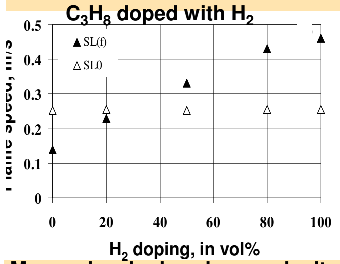
$(S_T/S_L)_{Exp}$ vs. $(S_T/S_L)_{Model}$

$(S_T/S_{L0})_{Exp}$ vs. $(S_T/S_{L0})_{Model}$

Hydrogen Influenced Propane Flames – Kido database



Turbulent flame speed S_T vs. u' for C_3H_8 mixtures. Experiment vs. Model predictions (using S_L, and in other two cases using S_{L0} but b) without, c) with Le term



Mean local burning velocity embedded with preferential diffusion, S_L, in comparison with the unstretched laminar flame speed, S_{L0}. Kido et al 1998.

Summary on Hydrogen Explosion

- ❖ **The hydrogen-hydrocarbon mixture is rendered less reactive for flame propagation with HC substitution**
  (Muppala et al 2006; Law and Kwon 2004; Kido et al 1998)

- ❖ **Influence of hydrocarbon (e.g., propane) is realizable beyond 20% by vol. in mixtures of HC-H_2 mixtures on turbulent flame speed**
  (Muppala et al 2006; Halter et al 2006; Kido et al 1998)

- ❖ **Experiments and analytical predictions showed that propane substitution to H_2-air mixtures moderates cell formation due to PDT and Darrieus-Landau (hydrodynamic) instabilities**
  (Law and Kwon 2004)

- ❖ **There is potential of containing (or at least retarding) the occurrence of DDT in confined structures with addition of hydrocarbons to hydrogen mixtures**
  (Abdel Aal 2005; Law and Kwon 2004)