**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

- Superadiabaticity 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


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

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

Lewis Number Effects – DNS investigations

- DNS by Trouvé and Poinset 1994 on lean H₂/O₂/N₂ flames
- and DNS of lean H₂ flame by Bell et al. 2006 (not depicted here), confirm the Le influence on turbulent flame speed, especially in lean H₂ 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

Preferential Diffusion and Lewis number Effects

- Stream Line
- Higher Diffusive Reactant: D₂
- Lower Diffusive Reactant: D₁

Unburned (Fuel/O₂/N₂)

In the case of CH₄ or H₂ mixtures, Fuel is D₁ and O₂ is D₂

In the case of C₂H₆ or C₃H₈ mixtures, Fuel is D₂ and O₂ is D₁

Lewis Number Effects – Russian database

- Case1: For lean (ϕ=0.5, Le=0.45) H₂ mixture, S₀₅ is 5 times lower as compared with a rich (ϕ=2.0, Le=1.9) H₂-air mixture, whereas the slope (Sₜ/u') shows the opposite behaviour and Sₜ is markedly higher for the former mixture at u'>1 m/s

- Case2: For very lean (ϕ=0.17, Le=0.4) H₂ mixture (not depicted here), S₀₅ is by more than 15 times lower as compared with the above rich case, while Sₜ for both cases are roughly equal
### 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 \( Le < 1 \).

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**Premixed Turbulent Combustion Model**

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

\[
\frac{A_T}{A} \approx \frac{S_T}{S_{L0}} = 1 + \frac{0.46}{Le} Re_t^{0.25} \left( \frac{u'}{S_L} \right)^{0.3} \left( \frac{p}{p_0} \right)^{0.2}
\]

\[
\frac{A_T}{A} = \text{Normalized turbulent flame surface area}
\]

\[
\frac{S_T}{S_{L0}} = \text{Normalized turbulent flame speed}
\]

\[
\frac{u'}{S_L} = \text{Turbulence-chemistry interaction}
\]

\[
\alpha = \text{single pre-constant} \quad Le = \text{Lewis number}
\]

\[
Re_t = \text{Turbulent Reynolds number} \quad p = \text{Operating pressure}
\]

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**Leading Point Concept -- Critically Curved Flamelets**

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

\[
T_r = T_u + \left( T_b - T_u \right)/Le
\]

The chemical time scale for the highest local burning rate is

\[
\tau_{cr} = \tau_c \frac{R_c}{S_{L0}} = \tau_c Le^{-1} \left( \frac{T_b}{T_r} \right)^{1.5} \exp \left( \frac{\Theta \left( T_b - T_r \right)}{2T_b \left( T_r - T_r \right)} \right) \rightarrow \tau_{cr} = \tau_c \frac{\max \{ u_c(t) \}_r \rightarrow \infty}{u_c(t)}
\]

\[
S_T = S_{L0} \left[ 1 + \frac{0.46}{\exp(Le - 1)} \left( \frac{T_r}{T_b} \right)^{0.25} \left( \frac{p}{p_0} \right)^{0.2} \right]
\]

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

(percived at the convex part (positive curvature) of the flamelet facing towards unburned gas)
Expanding Spherical Turbulent Flames – Kido database

**Hydrogen** (40 flames)

\[ \phi = 0.5 \text{ to } 0.95 \]

Measured data:

\[ \frac{S_L}{S_{L0}} = 1.0 \text{ to } 3.1 \]

mean local burning velocity / unstretched lamin. fl. speed

\[ S_L = f(\text{PD}/D_o) \]

Model predictions

\[
\frac{S_T}{S_{L}} = \left[ 1 + \frac{0.46 \exp(Le - 1) \cdot Re}{S_{L0}} \right] \quad (\text{without } PD \text{ effect})
\]

\[
\frac{S_T}{S_{L0}} = \left[ 1 + 0.46 Re \cdot u' \right]^{0.28} \quad (\text{without } Le (DT) \text{ effect})
\]

Spherical gaseous (H\(_2\)) explosion

Nakahara, Kyushu University, Personal communication 2006

**Correlation Plots for Hydrogen Flames – Kido database**

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

\[ \text{Le: } 0.393, 0.397, 0.402, 0.411 \]

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

\[ \text{Le: } 0.393, 0.397, 0.402, 0.411 \]

\[ \text{S}_L/\text{S}_{L0} = 2.7, 3.1, 3.3 \]

Higher the ratio, greater the influence of PD

The model predictions (RHS) deviate more for increased ratios.

**Hydrogen Influenced Propane Flames – Kido database**

\[ \text{C}_3\text{H}_8 \text{doped with H}_2 \]

\[ \text{Le} = 1.57, 1.30 \]

Turbulent flame speed \(S_T\) vs. \(u'\) for \(\text{C}_3\text{H}_8\) 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.**
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-H₂ 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 H₂-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)