



Aalto University  
School of Engineering

# Lecture 7: Laminar premixed flames

(related : Warnatz, Ch. 3, 5, 8, 12 )

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*Combustion Course, Spring 2019*

*April 2019, Otaniemi*  
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# Upcoming Sessions

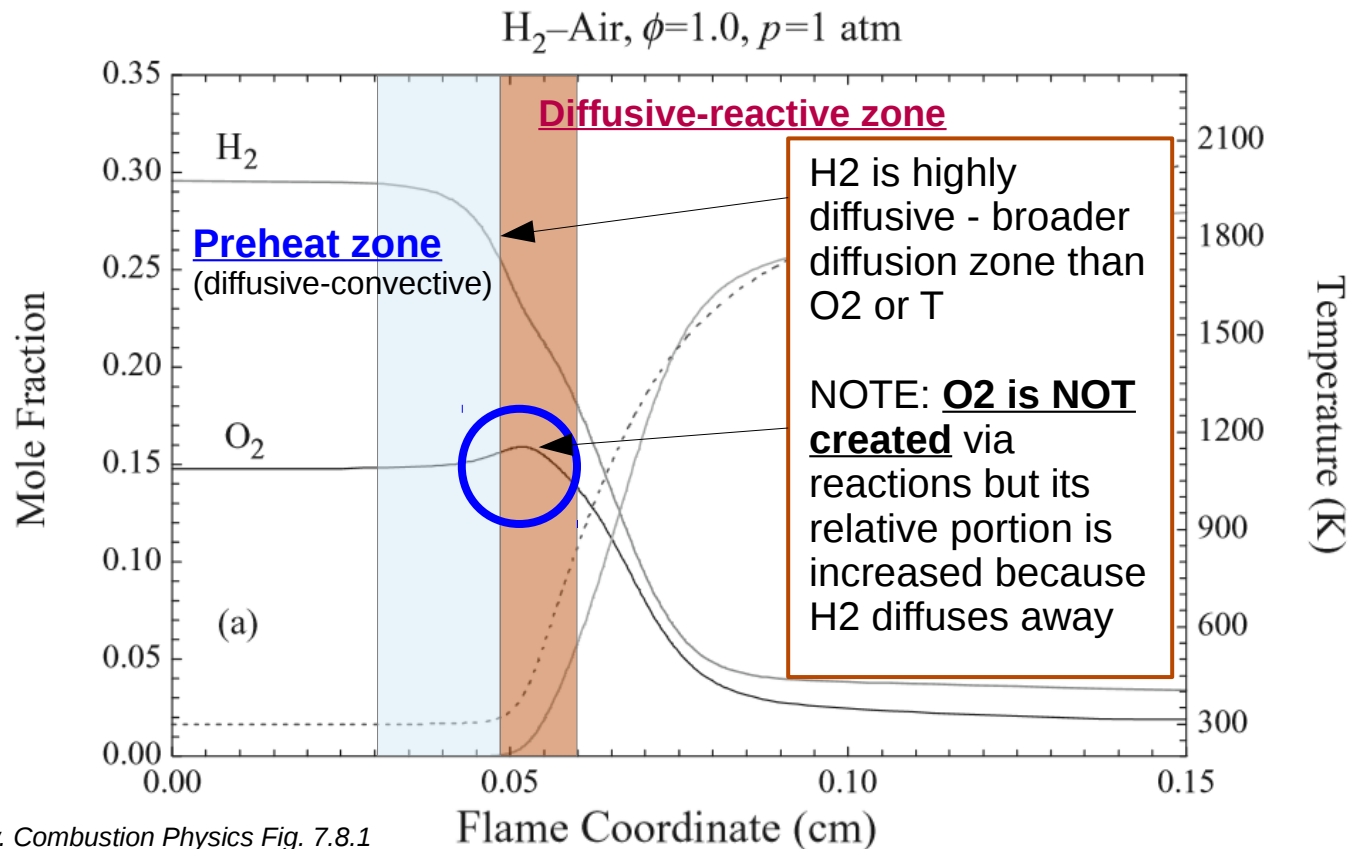
- Lecture 6: Laminar premixed flames
- Lecture 7: Details of laminar premixed flames
- Exercise 4 on theory and practice of laminar flame computations
- Exercise 5: Simple emission computations with Cantera
- My Course web interface for discussions and questions:  
<https://mycourses.aalto.fi/>

# Premixed (PM) flames (Recap)

- Reactants are perfectly premixed prior to ignition
    - all components necessary for the reaction are present in the fuel
    - to initiate reaction one has only to ignite the mixture
    - complete combustion
  - Formation of a propagation front
    - Front separates unburned from fully burned
    - self-sustaining
  - Targeted to lean conditions
    - complete combustion → “no” soot → no bright flame
    - Visibility depends on fuel: e.g. blue glow of the premixed bunsen flame originates from excited states of CH, C<sub>2</sub> (intermediate species in oxidization)
    - Lower combustion temperatures → lower No<sub>x</sub>
  - Applications : Gasoline and natural gas engines, modern gas turbines, explosions
-

# Chemical structure of PM flames (Recap)

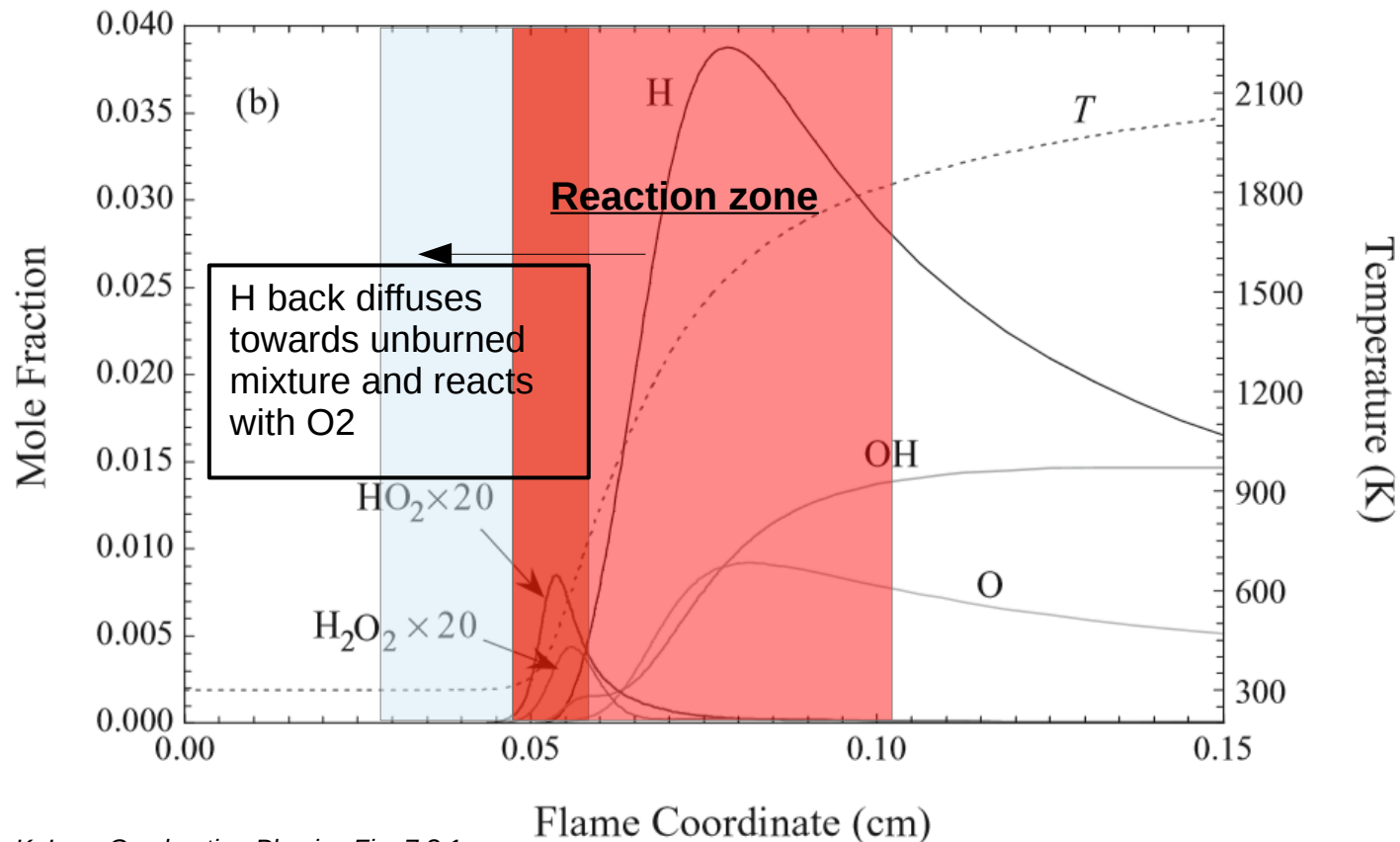
- Stoichiometric hydrogen flame



C. K. Law. Combustion Physics Fig. 7.8.1

# Chemical structure of PM flames (Recap)

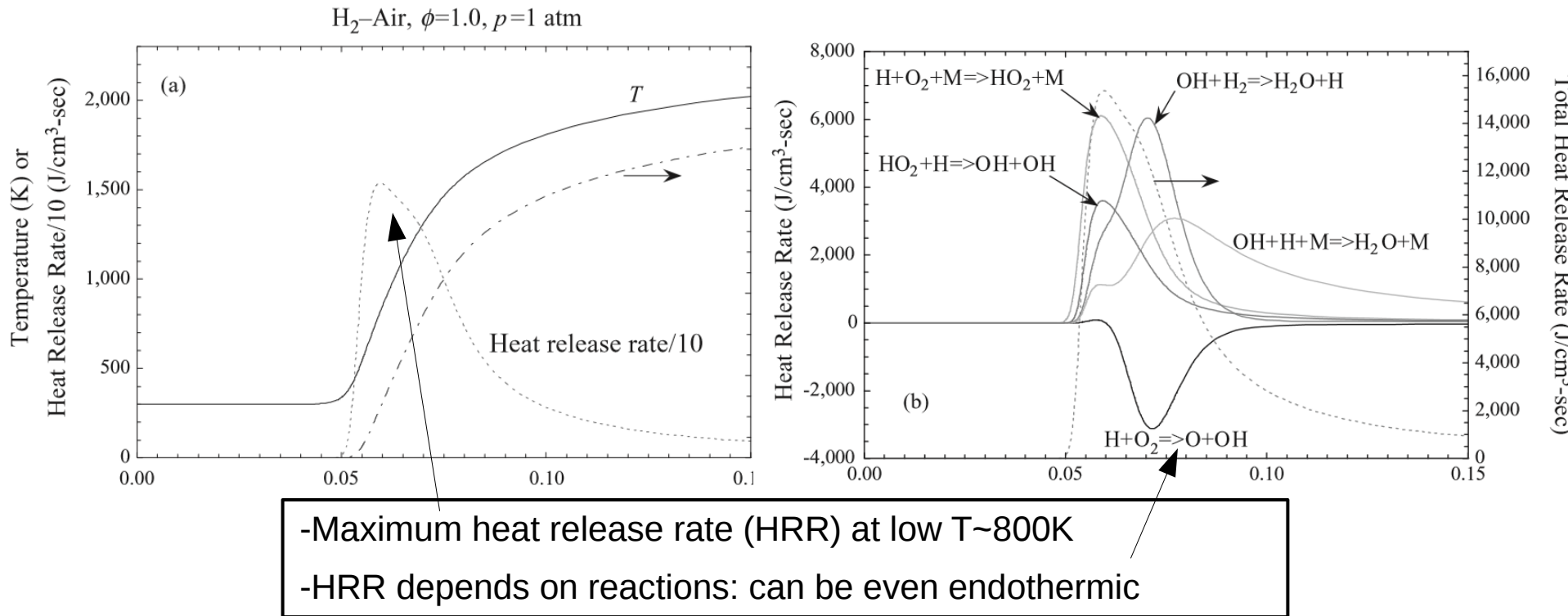
- Stoichiometric hydrogen flame



C. K. Law. *Combustion Physics* Fig. 7.8.1

# Chemical structure of PM flames

- Heat release in stoichiometric hydrogen flame (Recap)



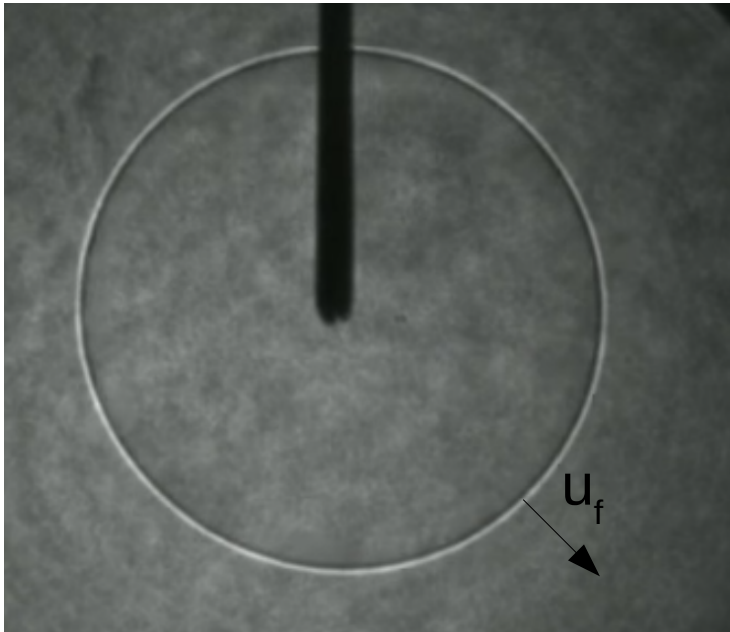
C. K. Law. *Combustion Physics* Fig. 7.8.2-3

# Chemical structure of PM flames (Recap)

- Important notes:
  - PM Flame has a finite thickness
  - Mass and heat diffusion are very important
  - Radicals and intermediate species can diffuse and initiate otherwise non-active reactions
  - Reactions take place throughout the flame thickness
  - Max heat release takes place at low T

# Laminar flame propagation

- Propagating flame front is an intrinsic feature of PM flames
- What influences to the propagation velocity ?
- How can we estimate this [“laminar flame speed”](#) ?



[https://www.youtube.com/watch?v=IwjiVdk\\_msA](https://www.youtube.com/watch?v=IwjiVdk_msA)



[https://upload.wikimedia.org/wikipedia/commons/e/e3/Blow\\_Torch\\_\(3257353199\).jpg](https://upload.wikimedia.org/wikipedia/commons/e/e3/Blow_Torch_(3257353199).jpg)



# Deflagration vs. detonation

- PM flame propagation is a wave phenomena
  - Subsonic = deflagration
  - Supersonic = detonation
- Deflagration waves:
  - pressure and density decrease across the wave
  - Deflagration wave considered near isobaric
- Detonation
  - pressure and density increase across the wave

# Deflagration vs. detonation

- PM flame propagation is a wave phenomena
  - Subsonic = deflagration
  - Supersonic = detonation

Most important in practical applications



- Deflagration waves:
  - pressure and density decrease across the wave
  - Deflagration wave considered near isobaric
- Detonation
  - pressure and density increase across the wave

# Governing Equations in Reactive Flows (Warnatz Ch. 12)

- Conservation of mass

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \vec{v}) = 0 . \quad (12.7)$$

- Species  $\rho_i = w_i \rho$

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div}(\rho_i \vec{v}) + \operatorname{div} \vec{j}_i = M_i \omega_i . \quad (12.8)$$

- Momentum

$$\frac{\partial(\rho \vec{v})}{\partial t} + \operatorname{div}(\rho \vec{v} \otimes \vec{v}) + \operatorname{div} \overline{\overline{p}} = \rho \vec{g} . \quad (12.9)$$

- Specific enthalpy

$$\frac{\partial(\rho h)}{\partial t} - \frac{\partial p}{\partial t} + \operatorname{div}(\rho \vec{v} h + \vec{j}_q) + \overline{\overline{p}} : \operatorname{grad} \vec{v} - \operatorname{div}(p \vec{v}) = q_r . \quad (12.12)$$

# Governing Equations in Reactive Flows (Warnatz Ch. 12)

- Conservation of mass

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \vec{v}) = 0 . \quad (12.7)$$

- Species  $\rho_i = w_i \rho$  Typically expressed in mass fractions

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div}(\rho_i \vec{v}) + \operatorname{div} \vec{j}_i = M_i \omega_i . \quad (12.8)$$

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Heat flux

e.g. radiation

# Governing Equations in Reactive Flows (Warnatz Ch. 12)

Driving force $\Rightarrow$ Flux $\Downarrow$	Velocity gradient	Temperature gradient	Concentration gradient
Momentum	Newton's law [ $\mu$ ]		
Energy		Fourier's law [ $\lambda$ ]	Dufour effect [ $D_i^T$ ]
Mass		Soret effect [ $D_i^T$ ]	Fick's law [ $D$ ]

**Fig. 5.8.** Fluxes and driving forces in transport processes (Onsager 1931, Hirschfelder et al. 1964)

# Governing Equations in Reactive Flows (Warnatz Ch. 12)

- **Heat flux consists of**

- Heat conduction (c)
- Dufour effect (negligible) (D)
- Flux due to mass diffusion (d)

$$\frac{\partial(\rho h)}{\partial t} - \frac{\partial p}{\partial t} + \text{div}(\rho \bar{v} h + \vec{j}_q) + \bar{p} : \text{grad } \bar{v} - \text{div}(p \bar{v}) = q_r. \quad (12.12)$$

$$\vec{j}_q = \vec{j}_q^c + \vec{j}_q^D + \vec{j}_q^d,$$

$$\vec{j}_q^c = -\lambda \text{grad } T$$

$$\vec{j}_q^D = \bar{M}RT \sum_i \sum_{j \neq i} \frac{D_i^T}{\rho D_{ij} M_i M_j} \left( \frac{w_j}{w_i} \vec{j}_i - \vec{j}_j \right)$$

$$\vec{j}_q^d = \sum_i h_i \vec{j}_i$$

Coefficient of thermal diffusion :  
important for H, H<sub>2</sub>  
at low  
temperatures  
(often omitted)

Binary diffusion coefficient :  
depend on concentrations  
and temperature

# Governing Equations in Reactive Flows (Warnatz Ch. 12)

- **Diffusion flux consists of**
  - Diffusion due to concentration (d)
  - Thermal diffusion (T)
  - Pressure diffusion (negligible) (p)

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div}(\rho_i \vec{v}) + \operatorname{div} \vec{j}_i = M_i \omega_i . \quad (12.8)$$

$$\vec{j}_i = \vec{j}_i^d + \vec{j}_i^T + \vec{j}_i^p$$

$$\vec{j}_i^d = \rho_i \vec{V}_i = \frac{\rho M_i}{M^2} \sum_{j \neq i} D_{ij}^{\text{mult}} M_j \operatorname{grad} x_j$$

$$\vec{j}_i^T = -D_i^T \operatorname{grad}(\ln T)$$

$$\vec{j}_i^p = \frac{\rho M_i}{M^2} \sum_{j \neq i} D_{ij}^{\text{mult}} M_j (x_j - w_j) \operatorname{grad}(\ln p)$$

*Multicomponent  
diffusion coefficient*

# Governing Equations in Reactive Flows (Warnatz Ch. 12)

- **Computing the multicomponent diffusion coefficient**

- From the kinetic theory of gases
- Very expensive
- Many theoretical and practical computational tricks needed
- Information (beyond course coverage) from Warnatz Ch. 5

$$L_{jk}^{00,00} = \frac{16T}{25p} \sum_{l=1}^K \frac{X_l}{m_j \mathcal{D}_{jl}} \{m_k X_k (1 - \delta_{jl}) - m_j X_j (\delta_{jk} - \delta_{kl})\}.$$

$$L_{jk}^{00,10} = \frac{8T}{5p} \sum_{l=1}^K X_k X_l (\delta_{jk} - \delta_{jl}) \frac{m_l (1.2C_{kl}^* - 1)}{(m_k + m_l) \mathcal{D}_{kl}}.$$

$$L_{jk}^{10,00} = L_{kj}^{00,10}.$$

$$L_{jk}^{01,00} = L_{kj}^{00,01} = 0.$$

$$L_{jk}^{10,10} = \frac{16T}{25p} \sum_{l=1}^K \frac{m_j}{m_k} \frac{X_j X_l}{(m_j + m_l)^2 \mathcal{D}_{jl}} \times \left\{ (\delta_{kl} - \delta_{jk}) \left[ \frac{15}{2} m_k^2 + \frac{25}{4} m_l^2 - 3m_l^2 B_{jl}^* \right] - 4m_k m_l A_{jl}^* (\delta_{kl} + \delta_{jk}) \left[ 1 + \frac{5}{3\pi} \left( \frac{C_{j,\text{rot}}}{R\xi_{jl}} + \frac{C_{l,\text{rot}}}{R\xi_{lj}} \right) \right] \right\}.$$

$$L_{jj}^{10,10} = -\frac{16m_j X_j^2}{R\mu_j} \left( 1 + \frac{10C_{j,\text{rot}}}{R\xi_{jj}} \right) - \frac{16T}{25p} \sum_{l \neq j}^K \frac{X_j X_l}{(m_j + m_l)^2 \mathcal{D}_{jl}} \times \left\{ \frac{15}{2} m_j^2 + \frac{25}{4} m_l^2 - 3m_l^2 B_{jl}^* + 4m_j m_l A_{jl}^* \right. \\ \left. \times \left[ 1 + \frac{5}{3\pi} \left( \frac{C_{j,\text{rot}}}{R\xi_{jl}} + \frac{C_{l,\text{rot}}}{R\xi_{lj}} \right) \right] \right\}.$$

$$L_{jk}^{10,01} = \frac{32T}{5\pi p C_{k,\text{int}}} \sum_{l=1}^K \frac{m_k A_{kl}^*}{(m_k + m_l) \mathcal{D}_{kl}} (\delta_{jl} + \delta_{jk}) X_k X_l \frac{C_{k,\text{rot}}}{R\xi_{kl}}.$$

$$L_{jj}^{10,01} = \frac{16}{3\pi} \frac{m_j X_j^2}{\mu_j C_{j,\text{int}}} \frac{C_{j,\text{rot}}}{R\xi_{jj}} + \frac{32TR}{5\pi p C_{j,\text{int}}} \sum_{l \neq j}^K \frac{m_j A_{jl}^*}{(m_j + m_l) \mathcal{D}_{jl}} X_j X_l \frac{C_{j,\text{rot}}}{R\xi_{jl}}.$$

$$L_{jk}^{01,10} = L_{kj}^{10,01}.$$



# Governing Equations in Reactive Flows (Warnatz Ch. 12)

- Alternative diffusion flux formulations
  - Mixture-average formulation

$$\vec{j}_i = - \boxed{D_i^M} \rho \frac{w_i}{x_i} \text{grad} x_i - D_i^T \text{grad} (\ln T) . \quad (12.25)$$

$$D_i^M = \frac{1 - w_i}{\sum_{j \neq i} x_j / D_{ij}}$$

Binary diffusion coefficient :

(Lennard-Jones potentials → Binary diffusion coefficients, see Lec 3)

# Governing Equations in Reactive Flows (Warnatz Ch. 12)

- **Alternative diffusion flux formulations**

- Define non-dimensional Lewis number for each specie :  $Le_i = \frac{\lambda}{\rho D_{im} c_p}$ .
- Use this to rewrite your conservation equations :

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) - \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h \right) = \nabla \cdot \left( \frac{\lambda}{c_p} \sum_{i=1}^{N_s} \left( \frac{1}{Le_i} - 1 \right) h_i \nabla Y_i \right),$$

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) - \nabla \cdot \left( \frac{\lambda}{Le_i c_p} \nabla Y_i \right) = \dot{\omega}_i, \quad i = 1, \dots, N_s.$$

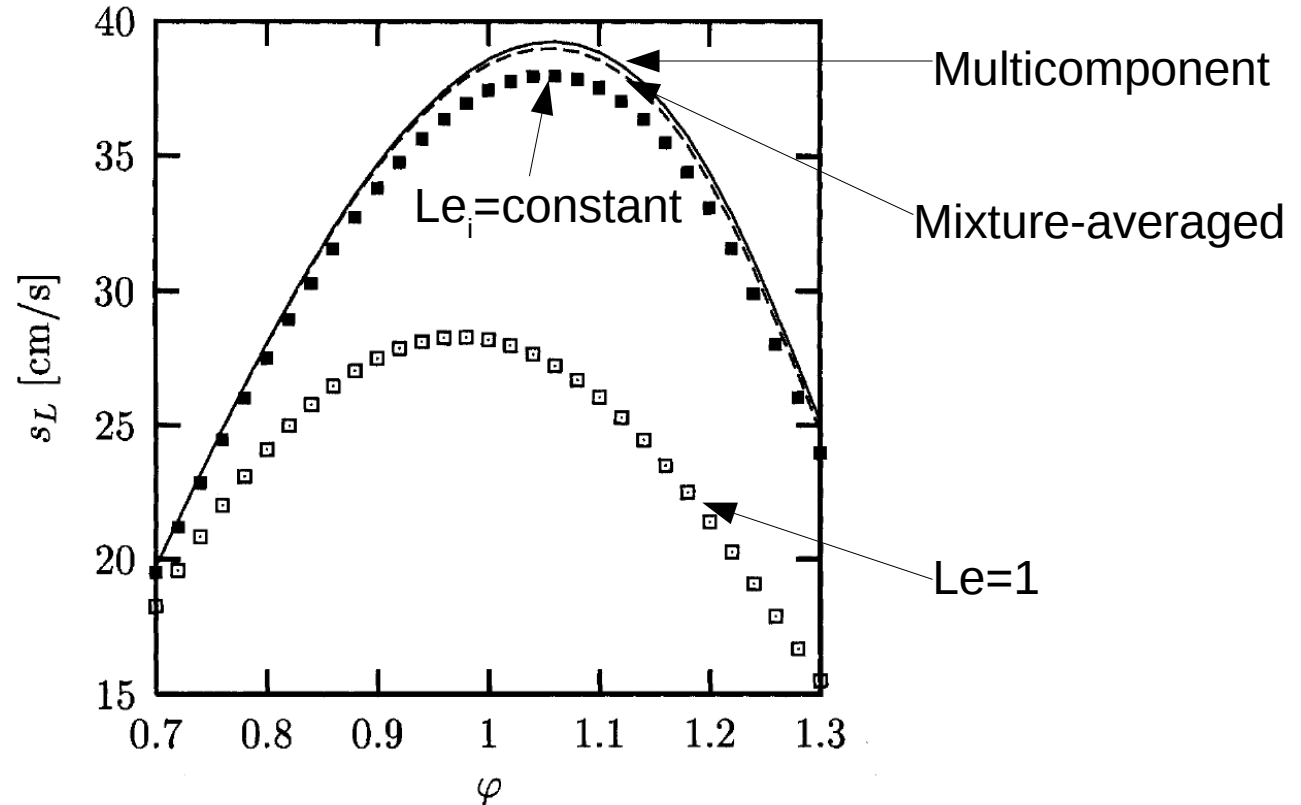
- Lewis number can be then species-wise constant, depend on temperature or Le = 1
- Le =1 is justified if turbulent mixing dominates the flow

# Governing Equations in Reactive Flows (Warnatz Ch. 12)

Driving force ⇒ Flux ⇓	Velocity gradient	Temperature gradient	Concentration gradient
Momentum	Newton's law [ $\mu$ ]		
Energy		Fourier's law [ $\lambda$ ]	Dufour effect [ $D_i^T$ ]
Mass		Soret effect [ $D_i^T$ ]	Fick's law [ $D$ ]

**Fig. 5.8.** Fluxes and driving forces in transport processes (Onsager 1931, Hirschfelder et al. 1964)

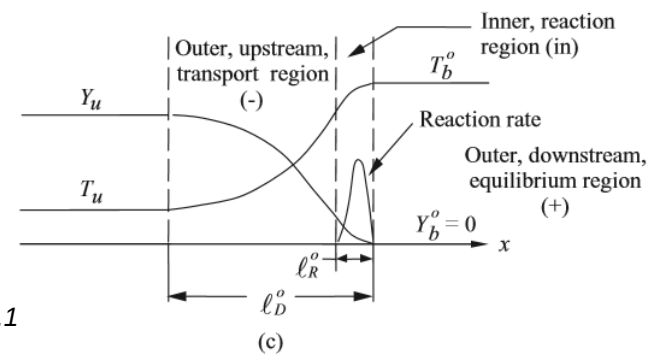
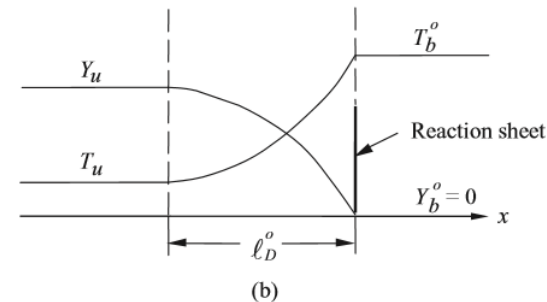
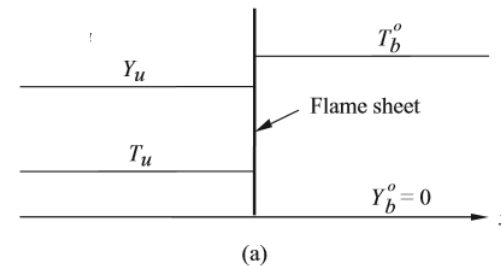
# Governing Equations in Reactive Flows (Warnatz Ch. 12)



Laminar flame speed of a methane flame with different diffusion models. Bongers et al. 2010

# Three levels of detail

- Flame sheet
  - Discontinuity
  - Conservation of mass and energy
  - Rankine-Hugoniot
  - Analytical analysis + combustion models
- Reaction sheet level
  - Includes the preheat zone
  - Finite thickness
  - Discontinuous reaction sheet
  - Analytical analysis + combustion models
- Complete structure
  - Fundamental understanding
  - Combustion models



C. K. Law. *Combustion Physics* Fig. 7.2.1

# Zeldovich's analysis of flame propagation (Warnatz Ch. 8)

- Solving the presented conservation equations is only possible via numerical methods
- Domain discretization for numerical methods should resolve the flame structure
- Numerical solution very CPU-intensive → modeling above 1D is mandatory
- Often the machine-crunched brute-force solution does not help us to understand the flame
- Simplified analytical analysis may give a lot of insight

# Zeldovich's analysis of flame propagation (Warnatz Ch. 8)

- Zeldovich and Kamenetskii developed the following analytical approach:
  - Assume 1D reacting flow
  - Assume steady-state flame (equivalent to steady flame front in bunsen burners)
  - One-step global reaction : Fuel (F)  $\rightarrow$  Products (P)
  - Global reaction rate  $r = -\rho w_F k = -\rho w_F \cdot A \cdot \exp(-E/RT)$
  - Multicomponent diffusion negligible and diffusion does not depend on location
  - The above results the following equations :

$$D \frac{\partial^2 w_F}{\partial z^2} - v \frac{\partial w_F}{\partial z} - w_F \cdot A \cdot \exp\left(-\frac{E}{RT}\right) = 0 \quad (8.1)$$

$$\frac{\lambda}{\rho c_p} \frac{\partial^2 T}{\partial z^2} - v \frac{\partial T}{\partial z} + w_F \frac{h_P - h_F}{c_p} \cdot A \cdot \exp\left(-\frac{E}{RT}\right) = 0 \quad (8.2)$$

# Zeldovich's analysis of flame propagation (Warnatz Ch. 8)

- Furthermore assuming  $Le = 1$  and the two equations become similar
- Change of variables and integration on both sides results single equation

$$\alpha \frac{d^2 \delta}{dz^2} - v \frac{d\delta}{dz} - \delta \cdot A \cdot \exp\left[-\frac{E}{R(T_b - \delta)}\right] = 0$$

$$\delta = T_b - T = [(h_P - h_F)/c_p] w_F$$

- We want to solve the profiles of temperature and species and particular velocity
- (steady state) + 2<sup>nd</sup> order ODE  $\rightarrow$  eigenvalue problem  $\rightarrow$  eigenvalue  $v_L = \sqrt{\frac{\alpha}{\tau}}$
- Mass burning flux (lam. Flame speed) is the fundamental property of the flame



# Zeldovich's analysis of flame propagation (Warnatz Ch. 8)

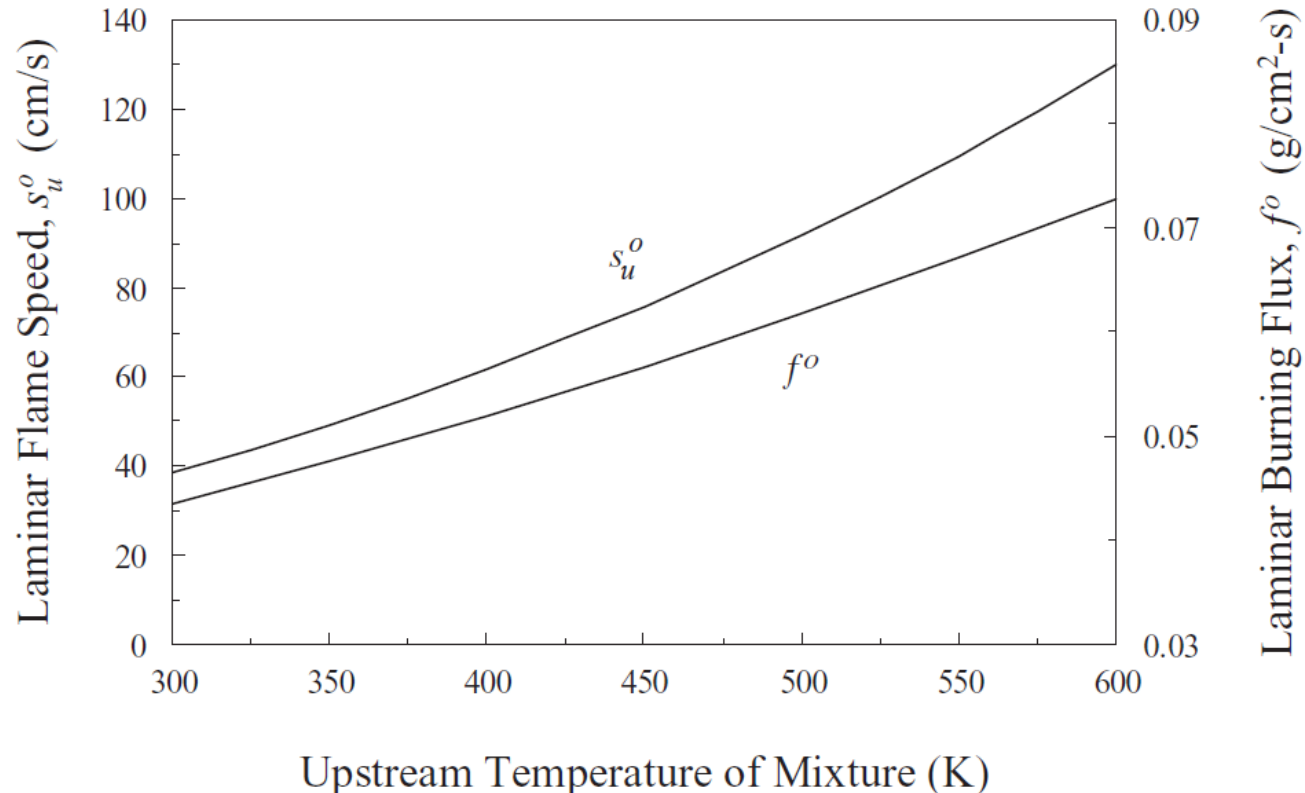
- Implications of Zeldovich's analysis  $v_L = \sqrt{\frac{\alpha}{\tau}}$   $\tau = 1/k = [A \cdot \exp(-E/RT)]^{-1}$ 
  - Laminar flame speed depends on the diffusivity  $\alpha$  and characteristic time of reaction  $\tau$
  - Flame propagation is caused by diffusive processes
  - Necessary gradients (wave) are sustained by the chemical reaction
- Furthermore, one can show that the flame thickness follows :  $\ell_F = \frac{\alpha}{v_L}$

# Laminar flame speed dependencies

- How does the mixture temperature effect?

# Laminar flame speed dependencies

- Mixture temperature effect : Stoichiometric CH<sub>4</sub>-air flame



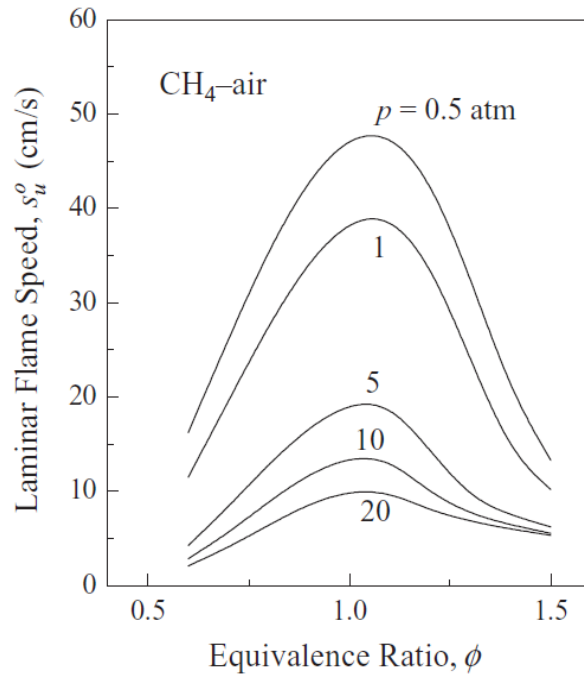
C.K. Law Combustion Physics : Fig. 7.7.12

# Laminar flame speed dependencies

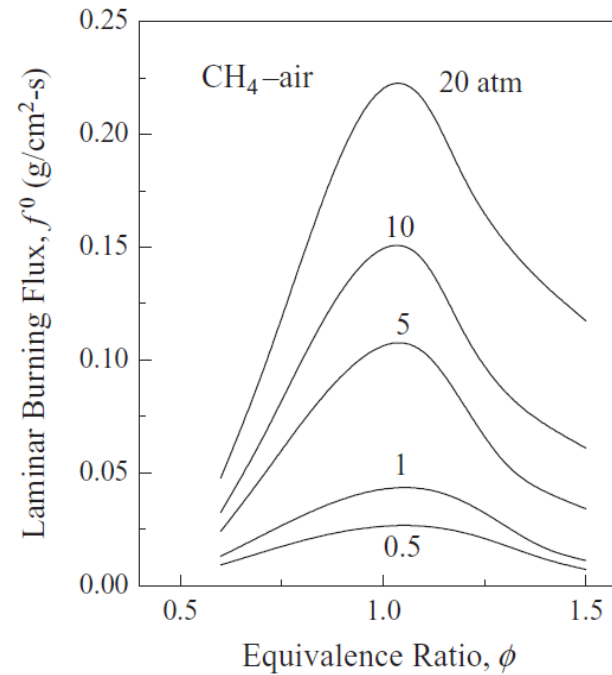
- How does the ambient pressure effect?

# Laminar flame speed dependencies

- Pressure effect on CH<sub>4</sub>-air flame : Laminar flame speed (a) and burning flux (b)



(a)

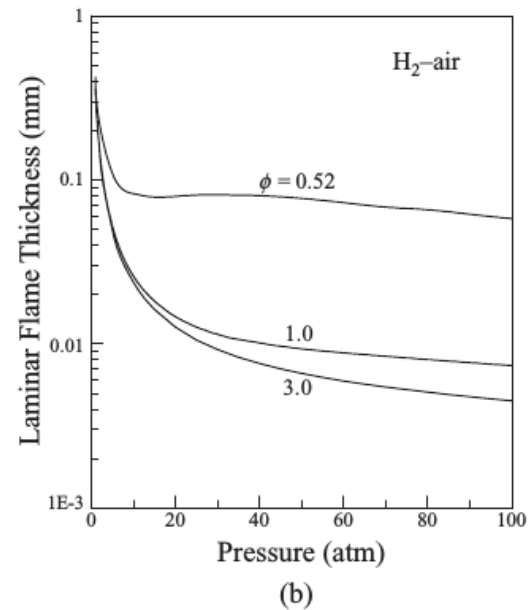
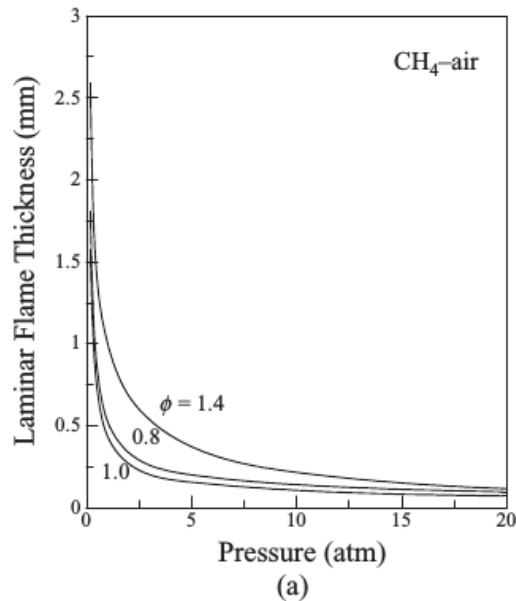


(b)

C.K. Law Combustion Physics : Fig. 7.7.7

# Laminar flame speed dependencies

- Pressure effect on flame thickness



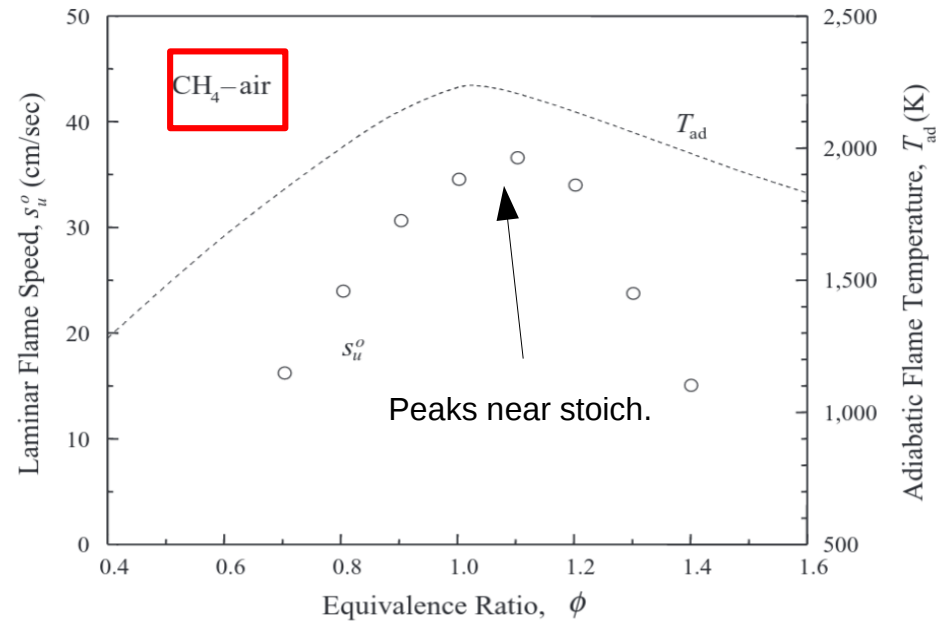
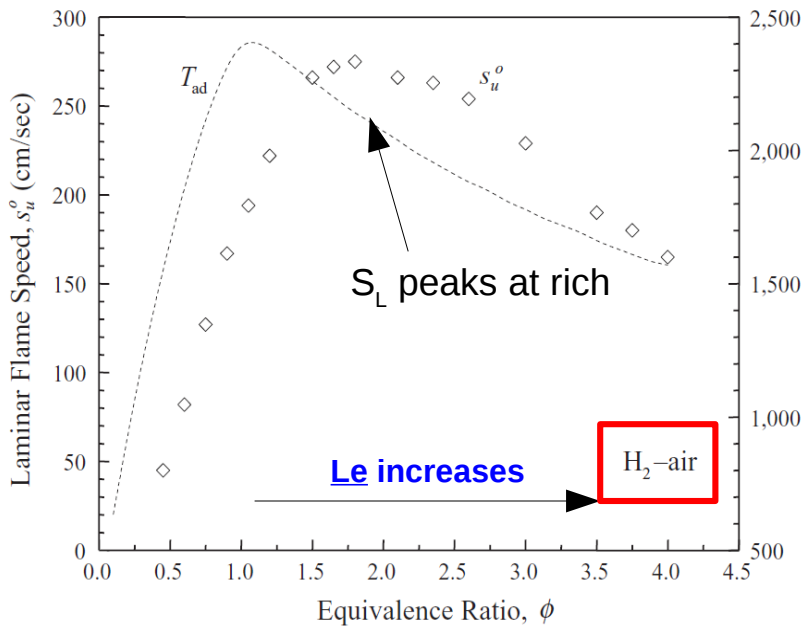
C.K. Law Combustion Physics : Fig. 7.7.11

# Laminar flame speed dependencies

- How about the fuel ?

# Laminar flame speed dependencies

- Adiabatic flame temperature and Lewis number effect
  - Higher heat of combustion → faster propagation
  - $S_L$  increases with  $T_{ad}$  and  $S_L \sim Le^{1/2}$

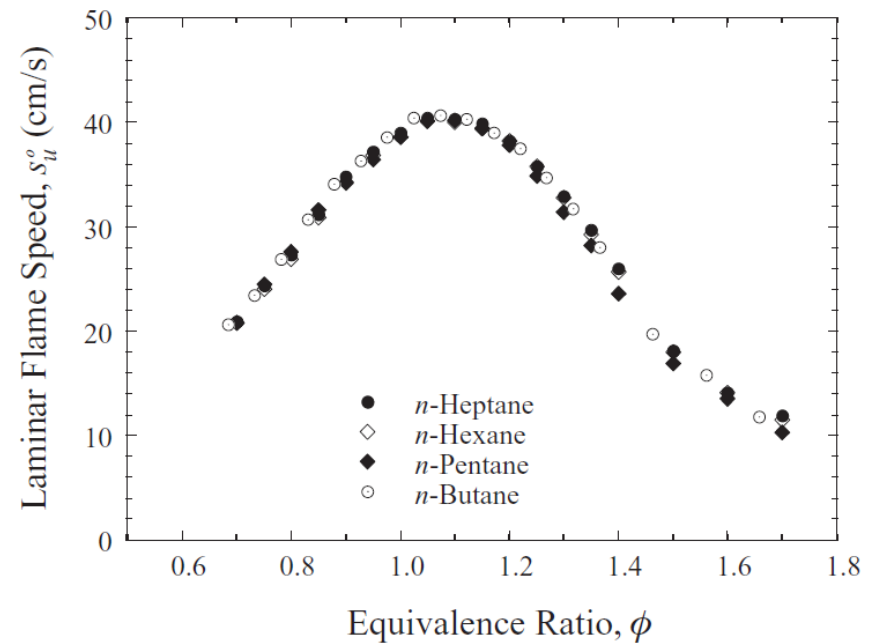
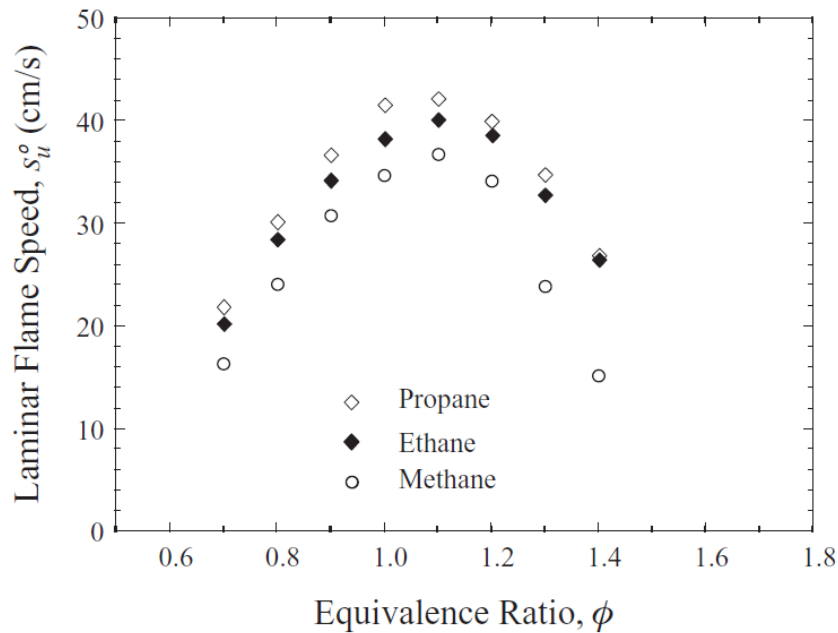


C.K. Law Combustion Physics : Fig. 7.7.2



# Laminar flame speed dependencies

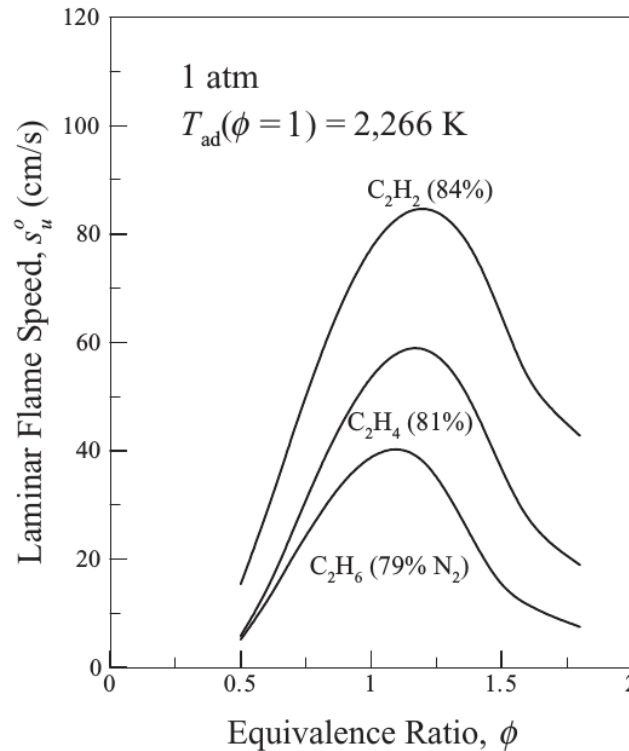
- Adiabatic flame temperature of the fuel dominates the flame speed
- Butane – Heptane share also very similar adiabatic flame temperature curves



C.K. Law Combustion Physics : Fig. 7.7.4

# Laminar flame speed dependencies

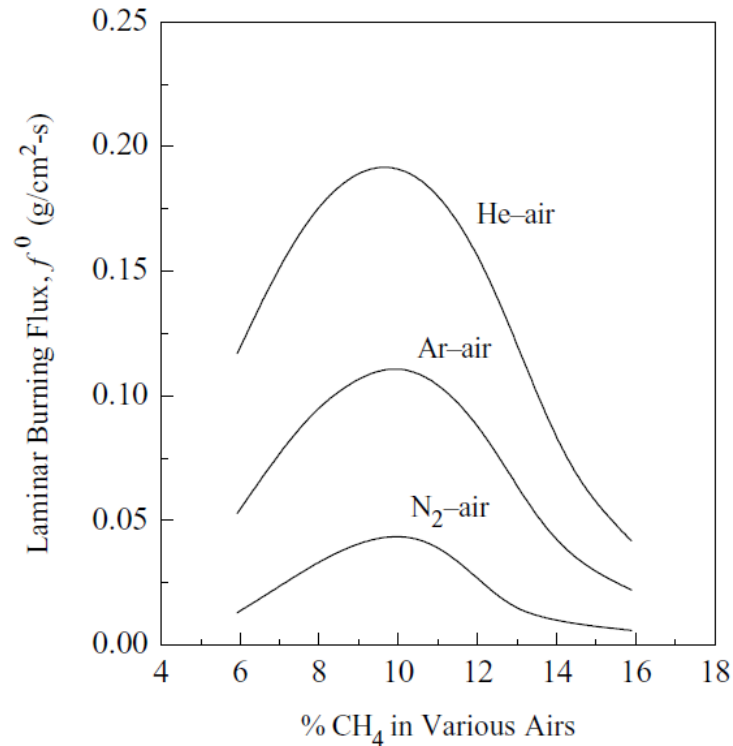
- However, molecular structure has a role, here fuels diluted to share same  $T_{ad}$  at stoich.



C.K. Law Combustion Physics : Fig. 7.7.6

# Laminar flame speed dependencies

- Transport property effect :  $v_L = \sqrt{\frac{\alpha}{\tau}}$



C.K. Law Combustion Physics : Fig. 7.7.13

# 1D flame calculations in practice

- Cantera has full capabilities to solve detailed chemistry in 1D
  - <http://www.cantera.org/docs/sphinx/html/cython/examples.html#one-dimensional-flames>
  - In particular we are interested in freely propagating adiabatic premixed flame :  
[http://www.cantera.org/docs/sphinx/html/cython/examples/onedim\\_adiabatic\\_flame.html](http://www.cantera.org/docs/sphinx/html/cython/examples/onedim_adiabatic_flame.html)
  - Note the choice of the mixture-averaged or multicomponent diffusion model
  - Cantera will discretize the 1D domain into N solution points
  - Resolution and time steps are controlled by the solver in run-time
  - However at high temperatures and pressures user has to modify the grid resolution criteria, time step and solver tolerances setup.