Wednesday: Non-premixed and Premixed Flames

Turbulent Combustion

Experiments and Fundamental Models

J. F. Driscoll, University of Michigan

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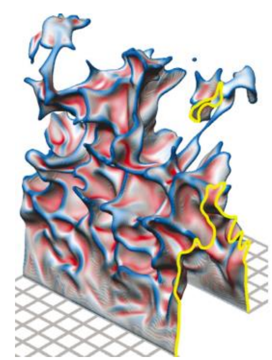
E. Hawkes,
Jackie Chen
T. Lu, C. K. Law
premixed



Bell, Day,
Driscoll
“corregated”
premixed

Outline for the week

Mon: **Physical concepts** faster mixing, faster propagation, optimize liftoff, flame surface density, reaction rate, PDF

Tues**:** **Kilohertz PLIF, PIV measurements of flame structure** - to assess models

Wed: **Non-Premixed and Premixed flames** - measurements, models
gas turbine example

Thurs: **Partially premixed flames -** and some examples

Fri: **Future challenges:** Combustion Instabilities (Growl) , Extinction

Assess JP-8 Chemistry ideas - of Hai Wang and others

"Lumped" Pyrolysis Model for JP-8 → butane, ethylene butene, propene, etc. → Detailed oxidation of each fuel

Step #1: JP-8 breaks down into simpler fuels - but without any oxidation ("lumped" = curve fit)

Step #2: the simpler fuels oxidize in ways that we understand

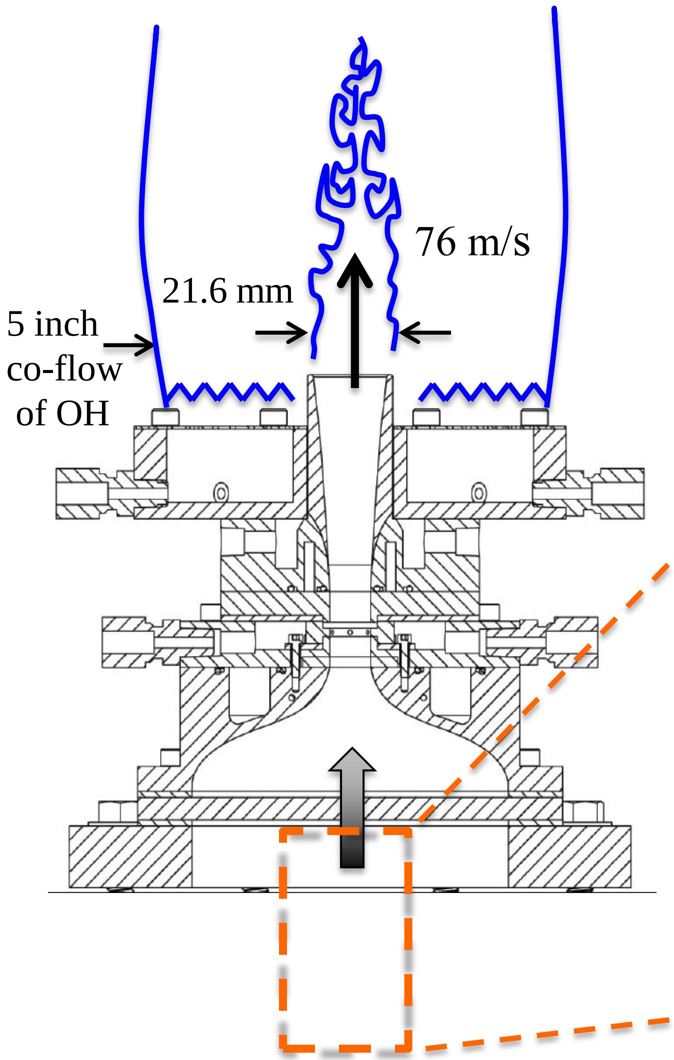
Shock tube studies give the Arrhenius constants for these many reactions

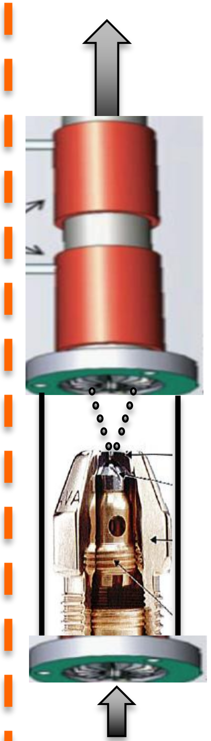
Need turbulent flame experiments to give us the temperature time-history = realistic residence time in turbulent flames that represent real engines

What are the limits to these approximations ?

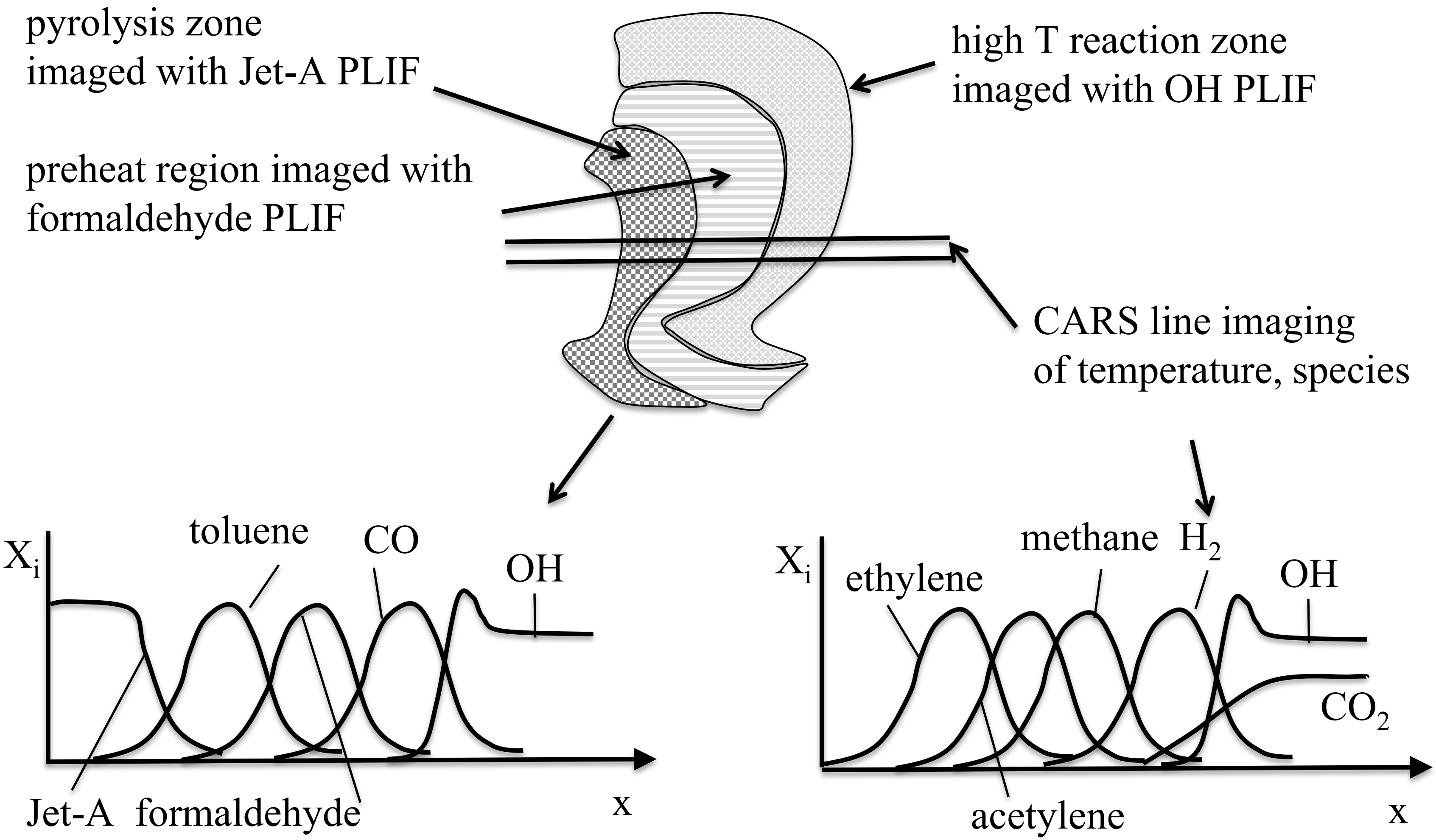
Michigan Hi-Pilot Burner - now operated on methane and JP-8

Vaporized JP-8 at Re_T up to 99,000





Imaging of pyrolysis layer - using vaporized JP-8 fuel

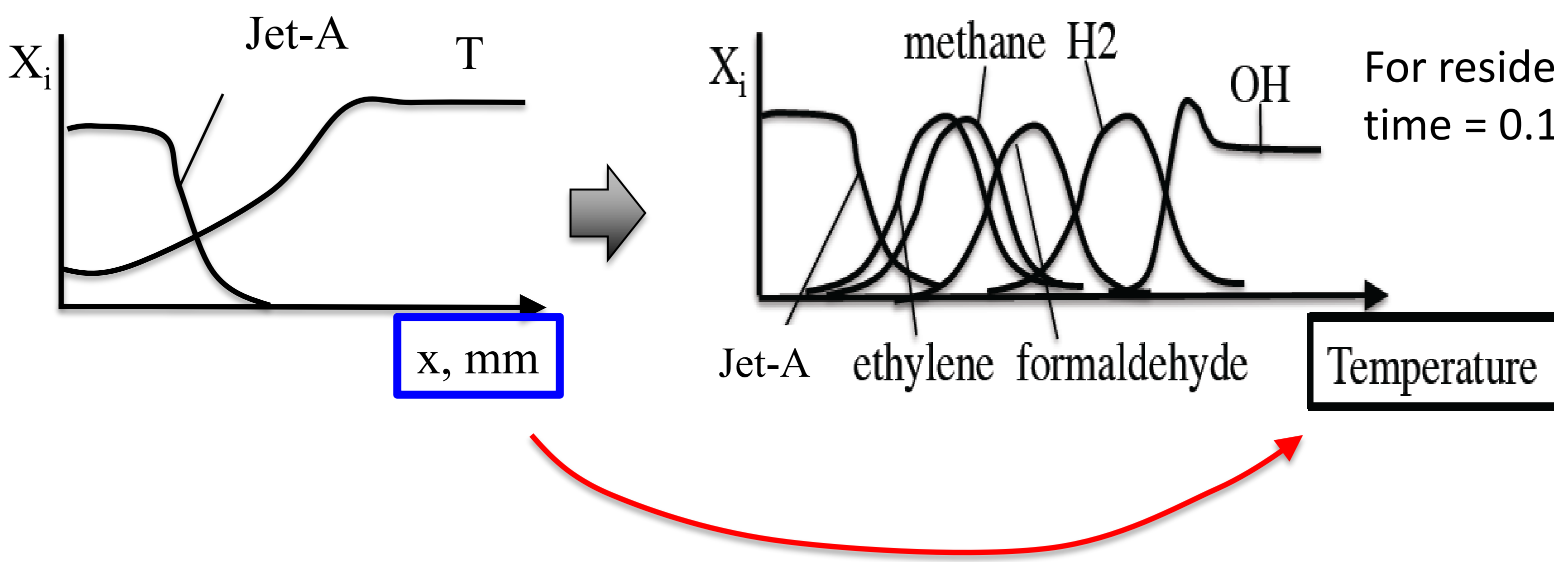


Fluorescence: 5 species (Michigan)   CARS: 9 species (Gord, Meyer)

Pyrolysis images – how to assess chemistry model ?

Each laser shot (at 10 Hz)

Simultaneously measure the profile of one species and temperature (CARS or LIF line imaging)



For residence time = 0.1 ms

b) Convert x axis to temperature axis and plot data from different runs

c) Simultaneous 2-D PLIF images of pyrolysis layer, preheat, reaction layer to measure residence time = thickness / normal velocity

Profiles of 14 species in a vaporized JP-8 flame -

can it be done ?

Species or temperature			Diagnostic		Location	Ref.
1	hydroxyl	OH	PLIF	2-D image	U. Michigan	1,7
2	formaldehyde	CH_2O	PLIF	2-D image	U. Michigan	1,7
3	JP-8	JP-8	PLIF	2-D image	U. Michigan	8-11
4	carbon monoxide	CO	LIF	line image	U. Michigan	12, 13
5	toluene	C_7H_8	LIF	line image	U. Michigan	14
	temperature	T	PLIF (2-line)	2-D image	U. Michigan	12
	temperature	T	nsec-CARS	line image	AFRL*	15-29
6	hydrogen	H_2	nsec-CARS	line image	AFRL	3
7	methane	CH_4	nsec-CARS	line image	AFRL	17, 19
8	carbon dioxide	CO_2	nsec-CARS	line image	AFRL	18
9	water	H_2O	nsec-CARS	line image	AFRL	17
10	carbon monoxide	CO	nsec-CARS	line image	AFRL	20
,12	nitrogen, oxygen	N_2, O_2	nsec-CARS	line image	AFRL	3
13	acetylene	C_2H_2	nsec-CARS	line image	AFRL	24
14	ethylene	C_2H_4	nsec-CARS	line image	AFRL	28, 29

“Evidence” that it can be done

8. LIF of kerosene: Linne, M. et al., Optical Diagnostics AIAA J. 45, 11, 2007.
9. Fluorescence spectroscopy of kerosene: Grisch, F., Applied Phys. B 116, 729, 2014.
10. PLIF of Jet-A: Hochgreb, S. et al., J. Prop. Power 29,4, 961, 2013.

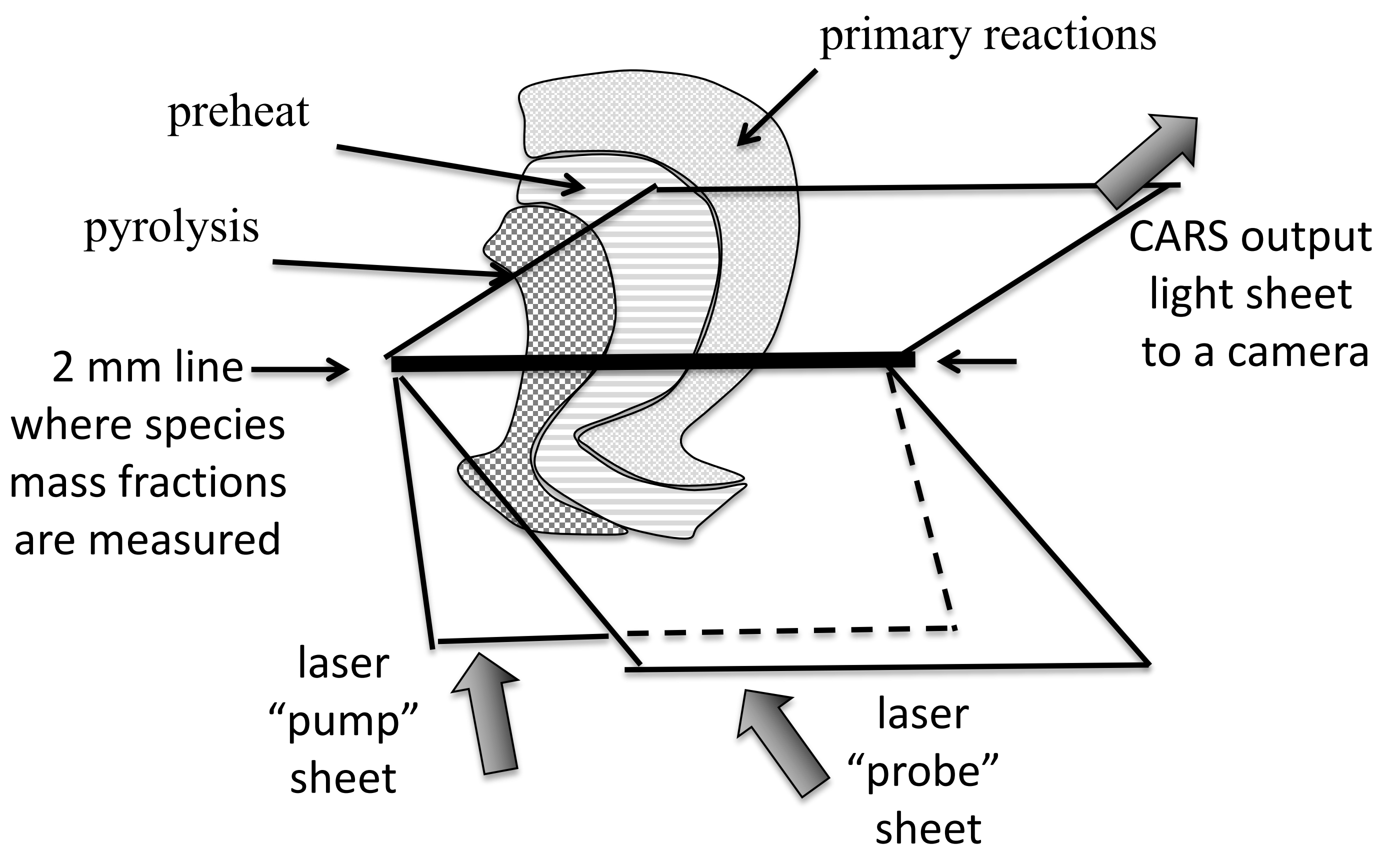
12. CO LIF: Barlow, R., Proc Comb Inst 32, 945, 2009
13. Temperature [CARS] and CO in Flames: Dreizler, A, Flow Turb Comb 90, 723, 2013.
14. LIF imaging of temperature [two line toluene] Sick, V et al, Proc Comb Inst 34, 3653

15. Gord, et al. 1-D thermometry in flames using CARS line imaging, Opt Let 36, 21
17. Gord, et al. [Review of CH4, H2, O2, N2 CARS] in PECS Vol. 36, p. 280
18. Gord, et al., CARS Temperature and CO2 Concentration, AIAA J. 41, 4, 679, 2003.

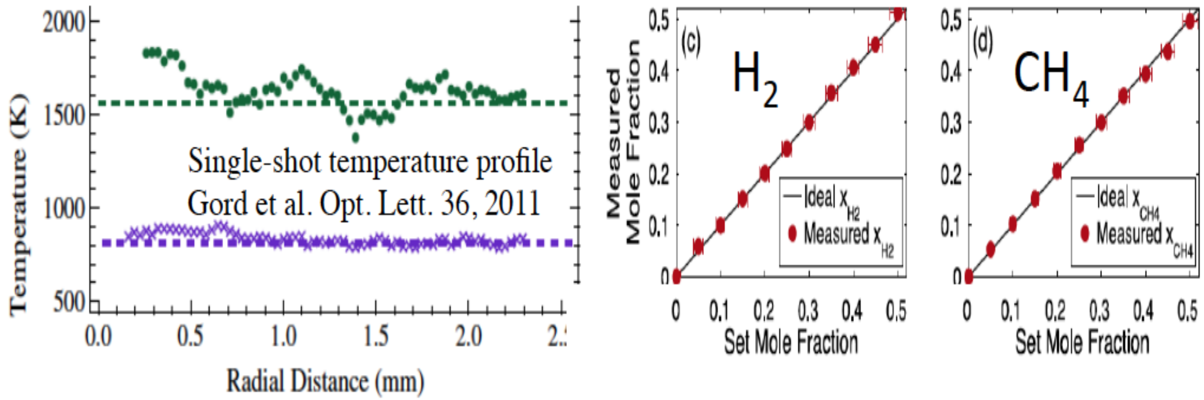
19. Meyer, T. et al [CH4, H2], Optics Lett 39, 23, 6608, 2014.
24. Gord, J. Detection of acetylene by CARS, Appl. Phys 87, 731, 2007.

MICHIGAN

Line CARS = coherent anti-Stokes Raman scattering - of Gord, AFRL



Results: line CARS at AFRL - Jim Gord



Preheat temperatures (3)   300K, 500 K, 700 K   (JP-8 cracks at 811 K)

Pressures (3):   1 atm. (years 1 and 2),   10 atm. (in year 3)

Reynolds number   80,000 for the highest case, is 16 times that of any previous burner

Future challenges - for Kilohertz laser diagnostics, LES and DNS

Highly unsteady combustion physics combustion instability ("growl")
structure of turbulent flames
how to apply Law's theory of flame stretch to highly turbulent flames ? Extinction, acceleration ?
does Landau instability dominate turbulent wrinkling ?
base of lifted jet flame – explain liftoff, blowout

Use kilohertz wisely, use LES wisely - look at the dynamics, don't just generate data !

Add heavy hydrocarbon chemistry to turbulent flame studies

DNS: Blanquart (Cal Tech), Poludnenko (NRL), Bell (LBL), Jackie Chen (Sandia)

Experiments: Ju (Princeton), Egolfopolous (USC)

Your airplane flight here was not powered by methane - but by Jet-A !

Best models of non-premixed turbulent flames

1. SSLF = steady strained laminar flamelet - Z & dissip rate (Peters, Pitsch)

2. FPV = flamelet progress variable – Z, c variables,
   no dissip rate (Moin)

1. PDF = method of Pope – parcels mix, mixing time eqn, Langevin eqn

1. CMC = Conditional Moment Closure – Bilger

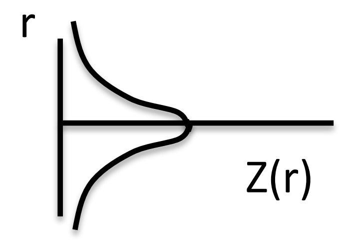
2. LEM = Linear Eddy Model – Kerstein, Menon

Simplest model of a turbulent non-premixed jet flame

Kuo, K. Principles of Combustion

1. Solve the laminar jet flame equations
2. **Replace molecular diffusivity D with turbulent diffusivity D_T**
3. Show that in a jet D_T is constant everywhere

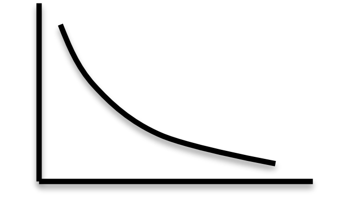
$$Z(x,r) = \frac{u(x,r)}{U_F} = \frac{3}{32}\,\frac{d_F}{x}\,\left(\frac{U_F\,d_F}{D_T}\right)\left(1+\frac{\xi^2}{4}\right)^{-2}$$



$$\xi = \left(\frac{r}{x}\right)\left(\frac{U_F\,d_F}{D_T}\right)\frac{\sqrt{3}}{8}$$

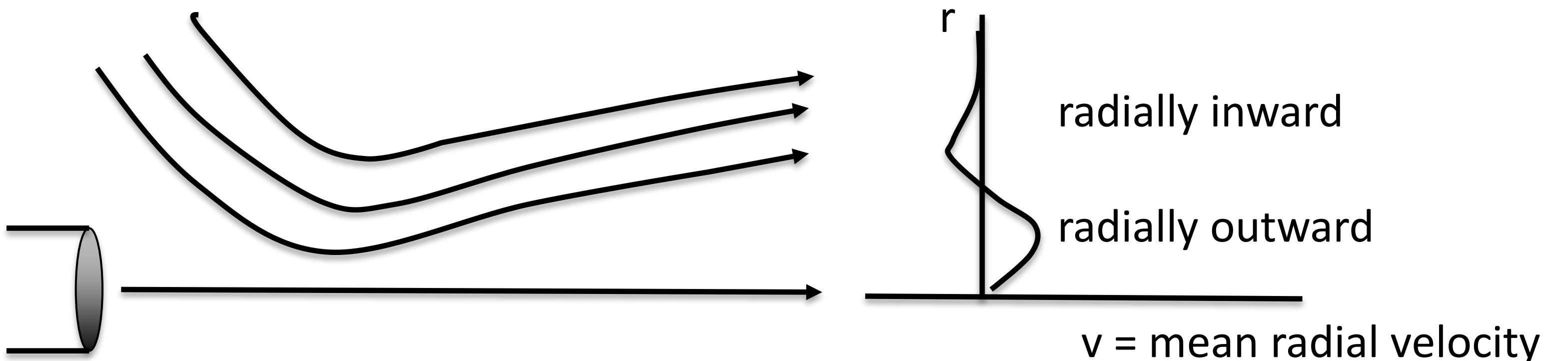
$$D_T \sim u'_{CL}\,L \sim U_{CL}\,L \sim \frac{U_F}{x/d_F}\,x \sim U_F\,d_F$$

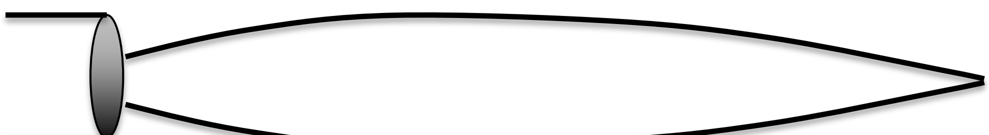
$$Z_{CL} = \frac{3}{32}\,\frac{d_F}{x}\,\left(\frac{U_F\,d_F}{D_T}\right)$$



Mean radial velocity (v) - in simple jet model

$$v = U_F \left(\frac{x}{d_F}\right)^{-1} \left(\xi - \frac{\xi^3}{4}\right)\left(1 - \frac{\xi^2}{4}\right)^{-2}$$





Flame location
Set $Z = Z_{st} = 0.55$
Plot eqn on previous slide

Flame length = flame location at r = 0, $L_f = d_F$ [constant/Z_{st}]

Next level of modeling non-premixed turbulent Jet Flame

– Unstrained flamelets Lockwood and Naguib, Comb. Flame 24, 109

he defines mixture fraction as f ; it is the same as Z

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_t \frac{\partial u}{\partial r}\right)$$ X - momentum

8 unknowns, 8 equations

$\tilde{u}$ $from\ x - mom\ eqn$

$\tilde{v}$ $from\ continuity\ eqn$

$\bar{Z} = \bar{f}$ $from\ \bar{f}\ eqn = \bar{Z}\ eqn$

$\tilde{g} = \widetilde{f'^2} = variance\ of\ f$

k $from\ k - eqn$

ε $from\ epsilon\ eqn$

$\bar{\rho}$ $from\ state\ relation$

$p = constant, assumed$

$$\rho u \frac{\partial \bar{f}}{\partial x} + \rho v \frac{\partial \bar{f}}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\mu_t}{\sigma_f}\frac{\partial \bar{f}}{\partial r}\right)$$ f - eqn

$$\rho u \frac{\partial k}{\partial x} + \rho v \frac{\partial k}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial r}\right) + \mu_t\left(\frac{\partial u}{\partial y}\right)^2$$

$$- C_D \frac{\rho^2 k^2}{\mu_t} + g C_\rho \frac{\mu_t}{\sigma_\rho}\frac{\partial \rho}{\partial x}$$ k equation

$$\rho u \frac{\partial \epsilon}{\partial x} + \rho v \frac{\partial \epsilon}{\partial y} = \frac{1}{r} \frac{\partial}{\partial r} \quad r \frac{\mu_t}{\sigma_\epsilon} \quad \frac{\partial \epsilon}{\partial r}$$

$$+ C_{\epsilon_1} C_D \rho k \left(\frac{\partial u}{\partial y}\right)^2 - \frac{C_{\epsilon_2}}{C_D} \rho \frac{\epsilon^2}{k}$$

epsilon equation

$$\rho u \frac{\partial g}{\partial x} + \rho v \frac{\partial g}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r \mu_t}{\sigma_g} \frac{\partial g}{\partial r} \right)$$

$$+ C_{g_1} \mu_t \left(\frac{\partial \bar{f}}{\partial y}\right)^2 - \frac{C_{g_2}}{C_D} \rho \epsilon_g$$

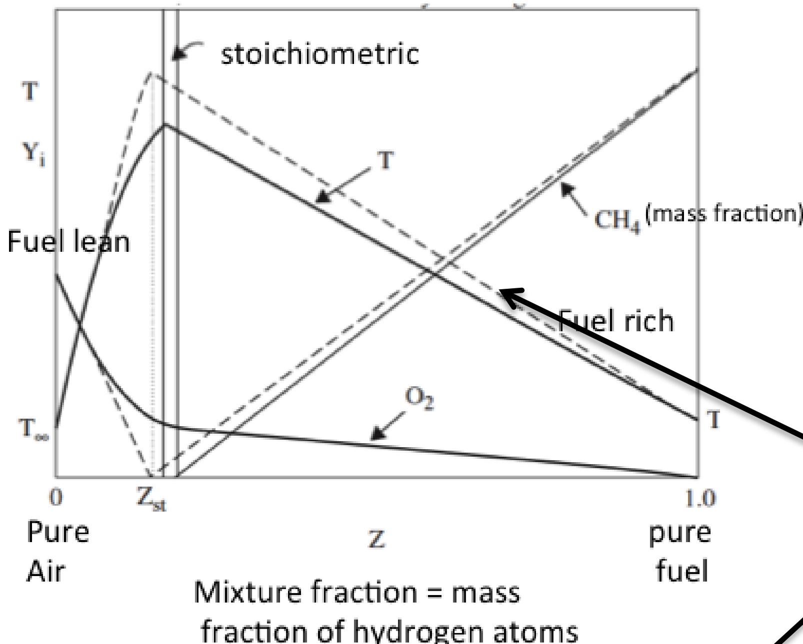
g – equation

Turbulent viscosity

$$\mu_t = C_D \rho \frac{k^2}{\epsilon}$$

Lockwood assumes unstrained Laminar flamelets

Closure = only need to solve eqn for mean mixture fraction Z, use lookup tables



Dotted lines = State relation from CHEMKIN for laminar unstrained (very low strain rate) flame

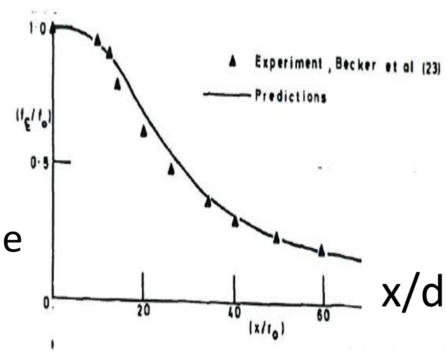
T(Z) = dotted line

$$\bar{T} = (\bar{Z},\overline{Z'^2}) = \int_0^1 T(Z) \quad P(Z,\bar{Z},\overline{Z'^2})\, dZ$$

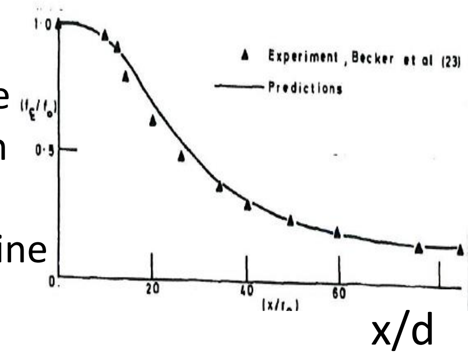
Note: no scalar dissipation rate appears for unstrained flamelets

RANS solutions – Lockwood and Naguib, Comb Flame 24, 109

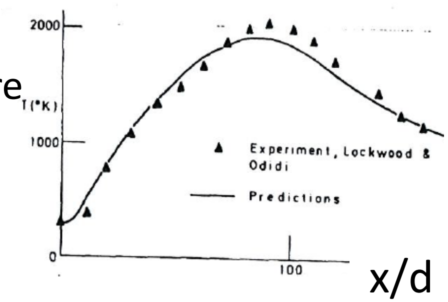
Mean
Velocity
On jet
centerline

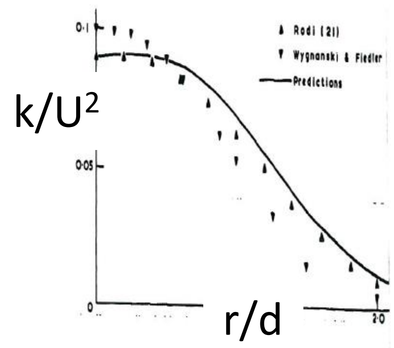


Mixture
fraction
On jet
centerline



Mean gas
temperature
On jet
centerline





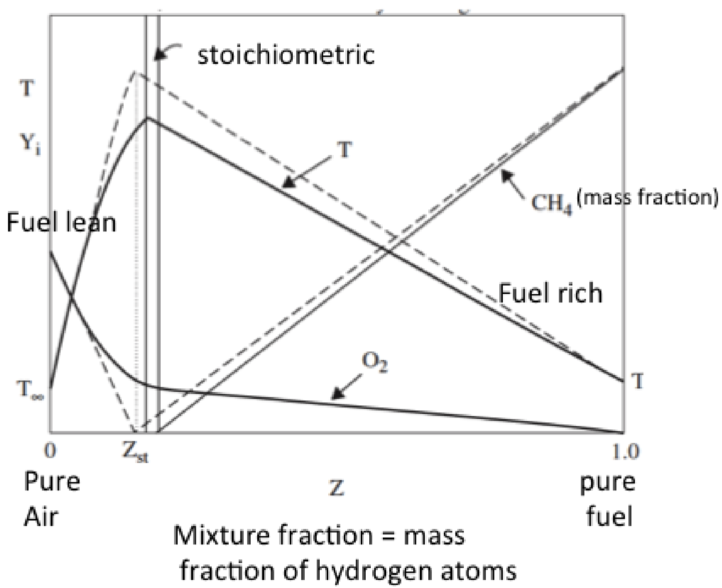
Problem – need to add **strained** flamelets = scalar dissipation rate
To correctly predict temperature, NOx, CO

Non-premixed flames - add strained flamelets - Peters

Flamelet lookup tables –
solve strained
counterflow flame

Scalar
Dissipation
rate

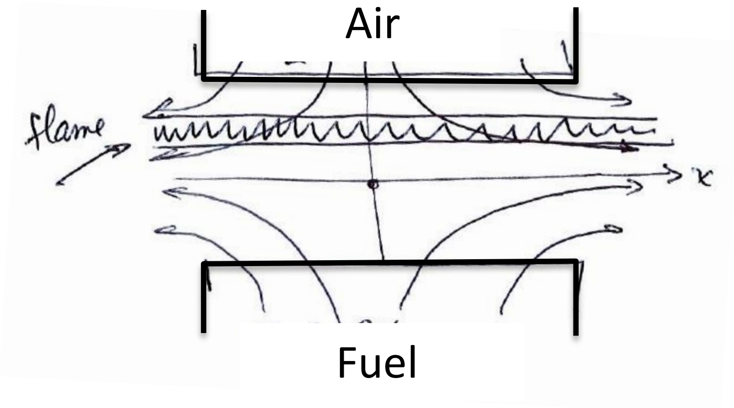
$$\chi = 2\,D\left[\overline{\left(\frac{\partial Z}{\partial x}\right)^2} + \overline{\left(\frac{\partial Z}{\partial y}\right)^2} + \overline{\left(\frac{\partial Z}{\partial z}\right)^2}\right]$$



Solid lines = state relations = CHEMKIN solutions to the **strained** flamelet equations with complex chemistry

Two variables are mixture fraction and scalar dissipation rate

Counter flow non-premixed flame (Peters)



$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$ So: u = ε x ; v = -ε y

Assume:

Laminar flow, fast chemistry
For simplicity, assume constant density
Velocity not disturbed by heat release
All species diffuse at same diffusivity D
Lewis number = 1, D = constant
Scalars only vary in the y (vertical) direction

$$\rho\, u\, \frac{dZ}{dx} + \rho\, v\, \frac{dZ}{dy} = \rho\, D\, \frac{d^2 Z}{dy^2} \quad \text{so}$$

$$(\epsilon\, x)\,[0] + (-\epsilon\, y)\,\frac{dZ}{dy} = D\, \frac{d^2 Z}{dy^2}$$

$$so: \quad (-\epsilon\, y)\frac{dZ}{dy} = D\, \frac{d^2 Z}{dy^2}$$

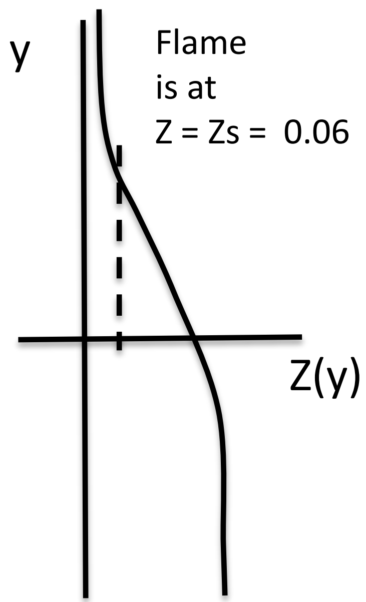
b.c.: y = oo, Z = 0, y = -oo, Z = 1

Solution to this equation is:

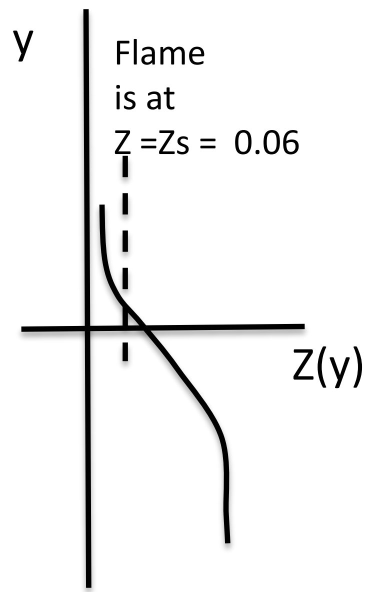
$$Z(y) = \frac{1}{2} - \frac{1}{2}\,\mathrm{erf}\left(\frac{y}{\sqrt{2D/\epsilon}}\right)$$

Scalar dissipation rate:

$$\chi = 2\,D\left[\overline{\left(\frac{\partial Z}{\partial x}\right)^2} + \overline{\left(\frac{\partial Z}{\partial y}\right)^2} + \overline{\left(\frac{\partial Z}{\partial z}\right)^2}\right]$$

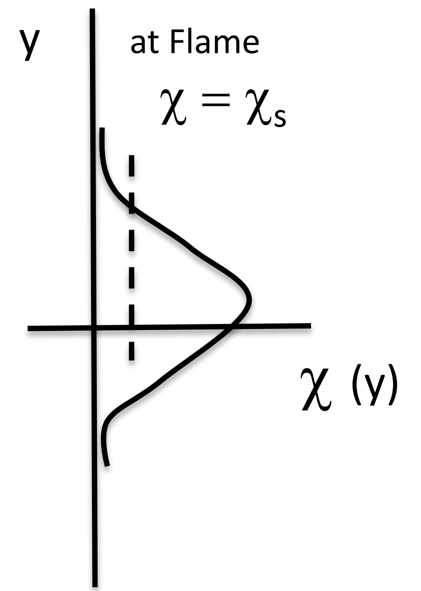


For low strain rate ε



For high strain rate ε

Larger gradient



χ_s = constant · ε

What is flame location $(y = y_f)$?

In solution for Z, set $Z = Z_s$ and solve for y

$$y_f = \sqrt{\frac{2\,D}{\varepsilon}}\,\mathrm{erf}^{-1}\,(1 - 2Z_s)$$

Flame location

Flame location:

Increasing D $\rightarrow$ y_f increases

Increasing ε or f_s $\rightarrow$ y_f decreases

Strength of a strained non-premixed counterflow flame

Strength of a non-premixed flame = mass flux of fuel at flame boundary

= J_F = mass of fuel consumed /sec per unit flame area

$$J_F = -\rho_F \, D \, \frac{\partial Y_F}{\partial y} \qquad \textit{Ficke's Law}$$

Use our state relation that says that Y_F is proportional to Z on the fuel side of flame

Take the derivative of the erf function formula for Z(y)

Plug in our formula for y = y_f at the flame front to get:

$$J_F = \rho_F \quad D^{1/2} \, \varepsilon^{1/2} \quad \cdot \quad constant$$

Stronger flame if strain rate ε is made larger and ε is Proportional to χ_{st}

How is scalar dissipation rate χ_s related to strain rate ε ?

Define scalar dissipation rate for this counter flow geometry

$$\chi = 2\, D \left[\overline{\left(\frac{\partial Z}{\partial y} \right)^2} \right]$$

Take the derivative of our erf function for Z(y) and

Plug into this formula, and plug in y = our formula for y_f at flame surface, to get:

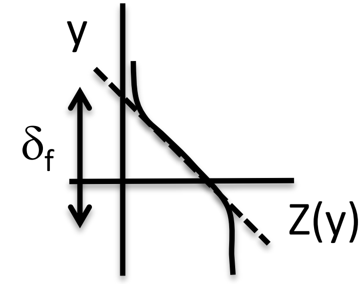
$$\chi_s = \varepsilon\ A \qquad where: \quad A = 4\, Z_s^2\, [erfc^{-1}(2\, Z_s)]^2$$

So the scalar gradient is related to velocity gradient

What is the thickness (δ_f) of a strained non-premixed flame ?

Define the thickness of a non-premixed flame to be:

$$\delta_f = \left(\frac{\partial Z}{\partial y}\right)^{-1}_{y=yf}$$



Take the derivative of our erf function for Z(y) and plug in our formula for y_f to get:

$$\delta_f = \sqrt{\frac{2\,D}{\chi_s}}$$

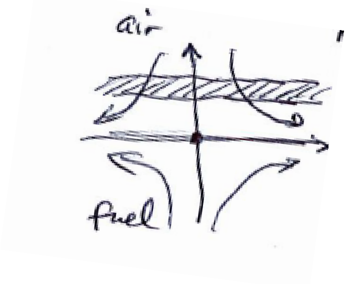
Flame gets thinner as you apply more strain

Example: if D = 1.0 cm^2/s = gas diffusivity near flame

if dissipation rate χ_s = 100 s^{-1}

Then flame thickness: δ_f = 1.4 mm

Flamelet assumption - of Peters adds **strain** to allow deviations from equilibrium chemistry



instantaneous T, Y_i are related to mixture fraction and dissipation rate in a turbulent flame in the same way they are related in a laminar counterflow flame with full chemistry

Steady non-premixed strained flamelet equation:

$$\cancelto{0}{\rho \frac{\partial Y_i}{\partial t}} = \frac{1}{2}\rho \chi \frac{\partial^2 Y_i}{\partial f^2} + \dot{\omega}_i$$

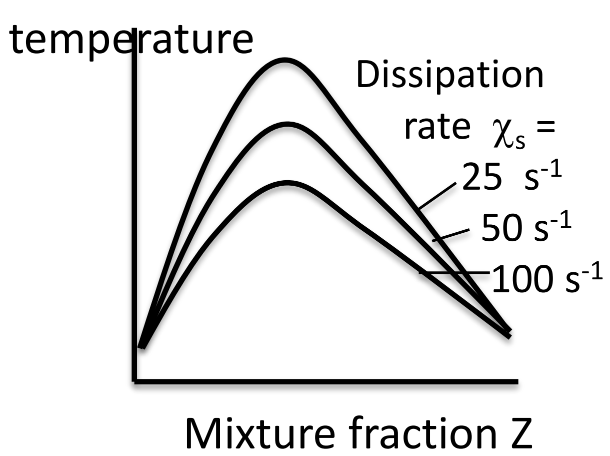
$$\bar{\chi}_s = C_\chi \left(\frac{\epsilon g}{k}\right)$$

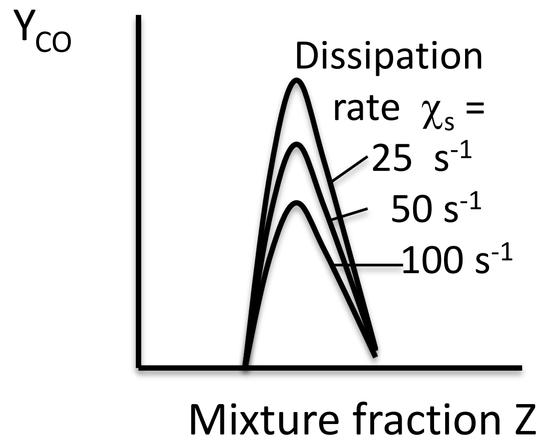
Solution yields state relations for all mass fractions, temperature, density as functions of Mixture fraction and Scalar dissipation rate

Now plug state relations into this to get mean values of temperature, density, mass fractions

$$\bar{Y}_{CO}\left(\bar{Z}, \overline{Z'^2}, \bar{\chi}, \overline{\chi'^2}\right) = \int_0^1 Y_{CO}(Z, \chi)\; P_1\left(Z, \bar{Z}, \overline{Z'^2}\right) P_2\left(\chi, \bar{\chi}, \overline{\chi'^2}\right) d\chi\, dZ$$

State relations - for a **strained** non-premixed counter flow laminar flamelet





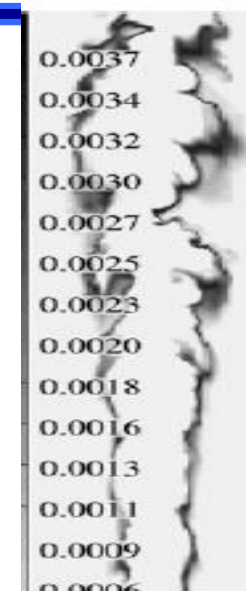
Generate plots above using CHEMKIN counter flow non-premixed flame solver

Larger velocity gradient (strain rate) = larger scalar gradient (scalar dissipation rate)

Larger dissipation rate → lowers the peak temperature,
alters the mass fractions of the species
reduces the chemical reaction rate until extinction occurs
improves prediction of CO, temperature, etc.

SSLF = Steady strained laminar flamelet LES model of Sandia Flame D by Janicka

Investigation of length scales, scalar dissipation, and flame orientation in a piloted diffusion flame by LES, A. Kempf J. Janicka PROCI 30 557



LES of Sandia flame D

Mixture fraction (Z) conservation eqn

$$\bar{\rho}\,\tilde{u}\,\frac{d\bar{Z}}{dx} + \bar{\rho}\,\tilde{v}\,\frac{d\bar{Z}}{dy} = \bar{\rho}\,D\,\frac{d^2\,\bar{Z}}{dy^2}$$

State relations from solutions to steady counter flow flamlet eqn
Mean mix fraction in subgrid = prop. to resolved scale gradients of Z
Variance of subgrid dissip. rate = prop. to resolved scale gradients
Assume a Beta function for P(Z), log-normal for P(χ). Mean quantities from:

$$\bar{Y}_{CO}\left(\bar{Z},\overline{Z'^2},\bar{\chi},\overline{\chi'^2}\right) = \int_0^1 Y_{CO}(Z,\chi)\;P_1\left(Z,\bar{Z},\overline{Z'^2}\right)P_2\left(\chi,\bar{\chi},\overline{\chi'^2}\right)d\chi\,dZ$$

state relation PDF

Janicka closure - for strained laminar flamelets

PDF of mixture fraction = Beta function, has mean and variance at each point
PDF of scalar dissipation rate = log normal shape, has mean and variance
At each (x,y,z) location we must compute the mean and variance of Z and χ

Mean mixture fraction - from Z conservation equation
Variance of mixture fraction - from “g” equation for scalar fluctuations

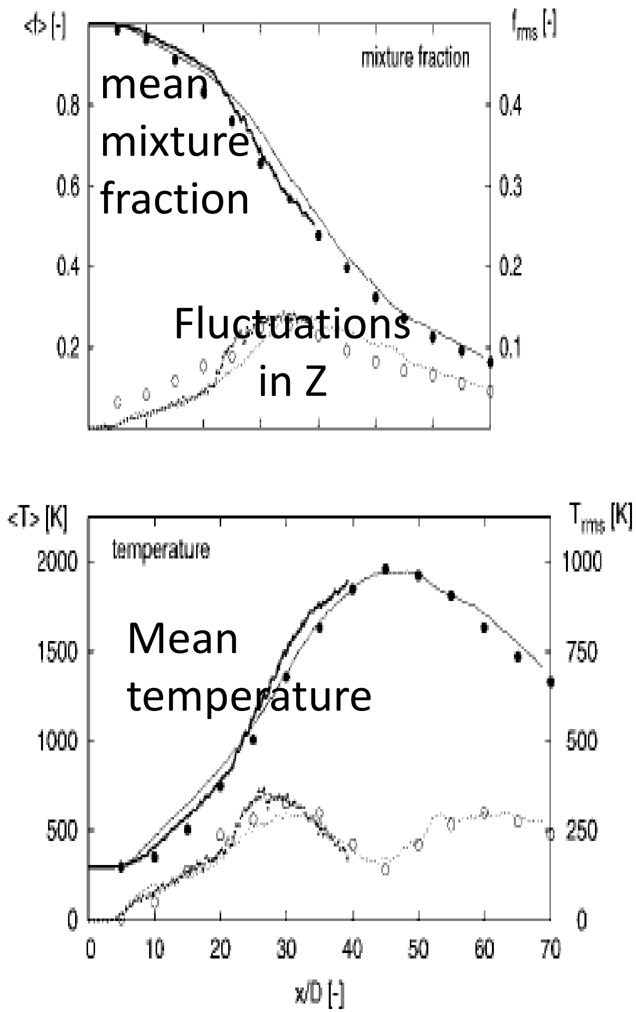
Mean scalar dissipation rate – assumed to be proportional to epsilon (dissipation rate of turbulent kinetic energy), multiplied by the variance of mixture fraction

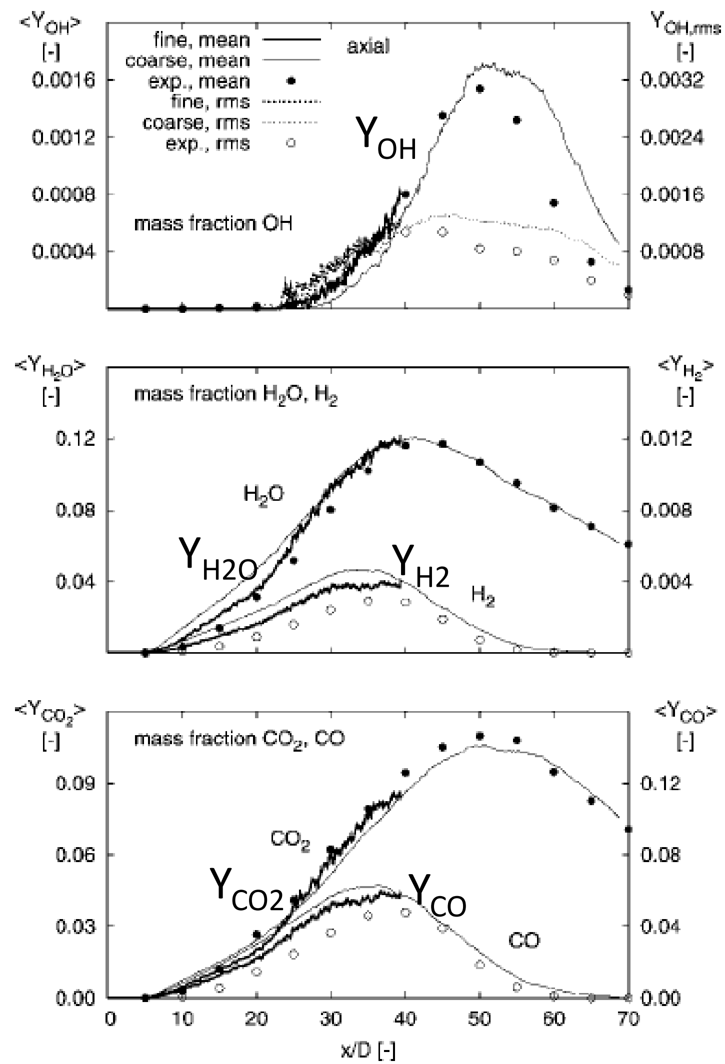
$$\bar{\chi}_{st} = \sigma_x \quad \varepsilon \quad \overline{Z'^2} \; / \; k$$

σ_x is a constant, k and ε come from the k and ε equations,

Variance of dissipation rate - assumed to be zero in FLUENT, others use an assumed algebraic equation

Janicka - SLF steady laminar flamelet model of Sandia Jet Flame D, PROCI 30 557





Janicka SLF LES, continued

PDF of scalar dissipation rate
Computed = bars
Measured = dots

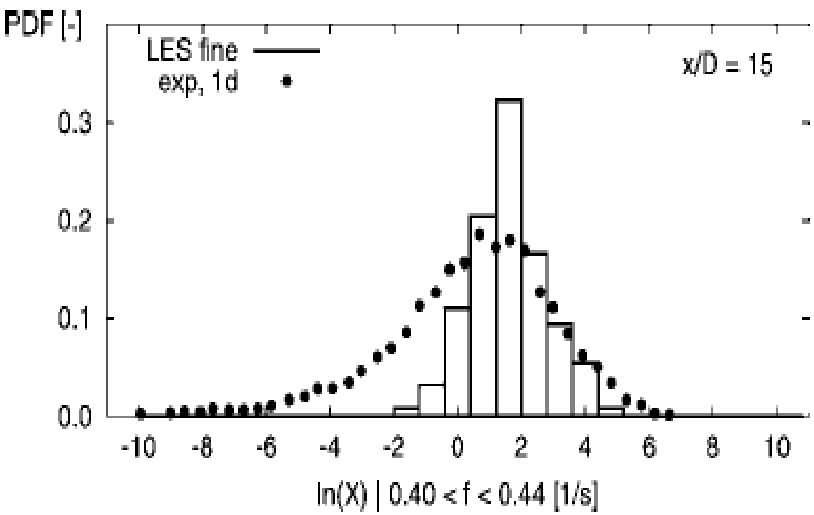


Fig. 9. The PDF of the resolved scalar dissipation rate. This quantity is expected to be log-normally distributed. Comparison of LES-data (1d) to experimental 1d-data.

Conclude: the steady laminar flamelet LES adequately simulates

the non-premixed combustion in Sandia jet flame D

except for H2 and CO on the fuel rich side – it is a little off

Flamelet progress variable (FPV-LES) model - compared to Barlow's measurements in a non-premixed jet flame

C. Hasse, "LES flamelet-progress variable modeling and measurements of a turbulent partially-premixed dimethyl ether jet flame" Comb Flame 162, 3016

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Z}) + \nabla\cdot(\bar{\rho}\,\tilde{\mathbf{u}}\,\tilde{Z}) = \nabla\cdot\left[\left(\bar{\rho}D_Z + \frac{\mu_t}{Sc_t}\right)\nabla\tilde{Z}\right]$$

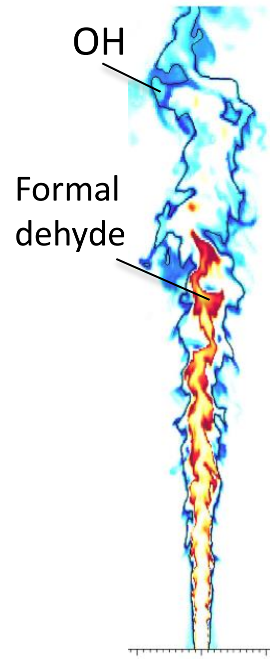
$$\widetilde{Z''^2} = C_{\widetilde{Z''^2}}\,\Delta^2\,|\nabla\tilde{Z}|^2$$

Replace scalar dissipation rate with a new progress variable Y_c

Progress variable: $Y_c = Y_{H2} + Y_{H2O} + Y_{CO} + Y_{CO2}$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_C) + \nabla\cdot(\bar{\rho}\,\tilde{\mathbf{u}}\,\tilde{Y}_C) = \nabla\cdot\left[\left(\bar{\rho}D_{Y_C} + \frac{\mu_t}{Sc_t}\right)\nabla\tilde{Y}_C\right] + \overline{\dot{\omega}}_{Y_C}$$

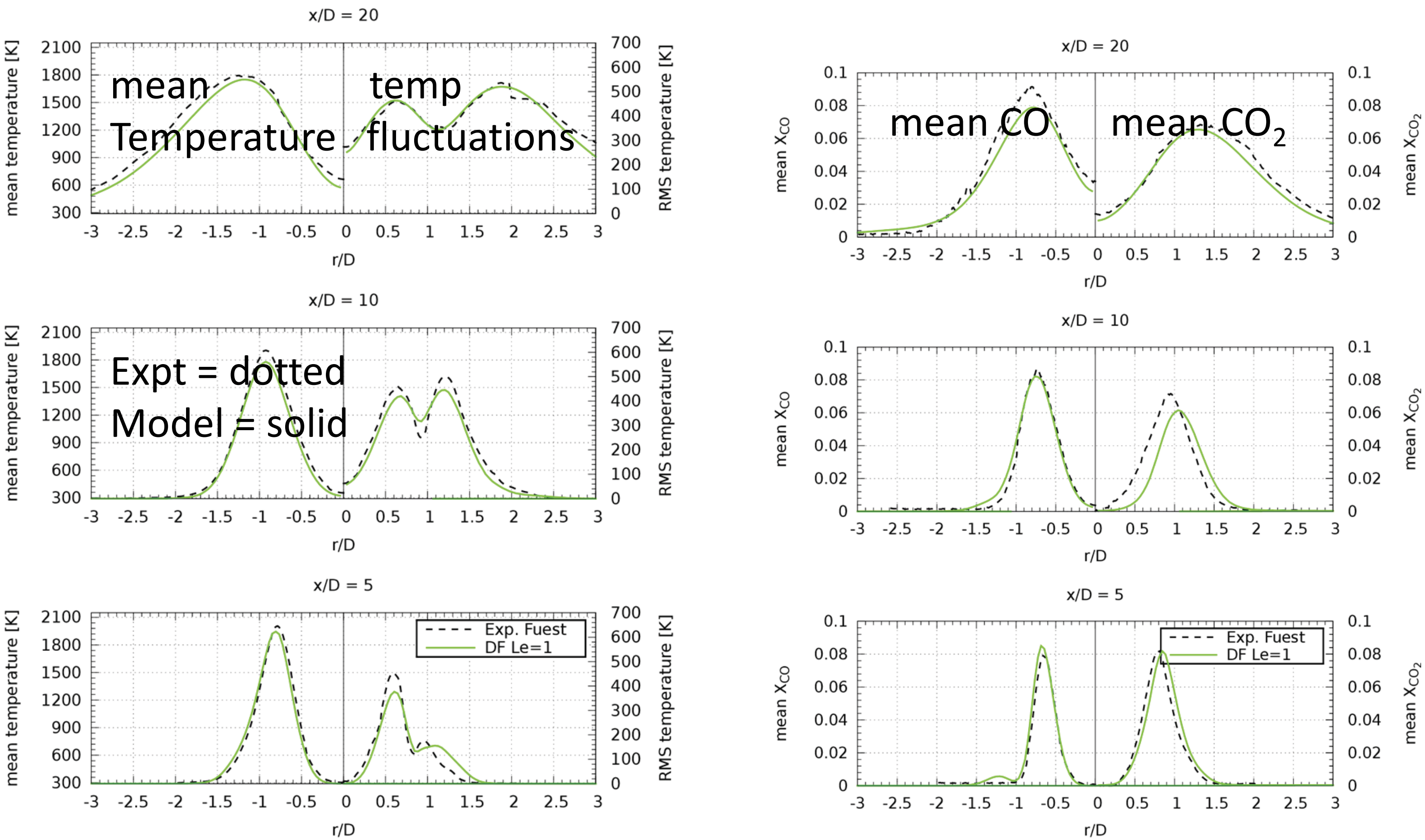
A presumed β-shaped filtered density function (FDF) is used to integrate the mixture fraction, and a δ-FDF is applied for the normalized progress variable to account for non-resolved fluctuations. Using a δ-FDF means that no subgrid closure is employed for the normalized progress variable. For the integration process, the nor-



LES of Hasse

Experiment Sandia flame D

LES – FPV model of Hasse (Frieberg) agrees with Sandia measurements



Conclude: the Flamelet Progress Variable (FPV)m odel gives good agreement with measurements for major species and CO. NO was not attempted

Good Measurements – of non-premixed turbulent combustion

See TNF website http://www.sandia.gov/TNF/

Single point Raman/Rayleigh/LIF data for f, T, N2, O2, CH4, CO2, H2O, H2, CO, OH, NO and velocity

Barlow, R. S., Frank, J. H., A. N. Karpetis, and Chen, J.-Y., "Piloted Methane/Air Jet Flames: Scalar Structure and Transport Effects," Combust. Flame 143:433-449 (2005).

Masri, A., Dibble, R.,Barlow, R., Structure of Turbulent Nonpremixed Flames Revealed by Raman-Rayleigh-LIF Measurements', Prog. Energy Combust. Sci., 22:307-362 (1997).

Barlow: Non-premixed piloted jet flame

in Comb Flame 143, 433 and

TNF website http://www.sandia.gov/TNF/

"Piloted methane/air jet flames: Transport effects and aspects of scalar structure"

Single point Raman/Rayleigh/LIF measurements of f, T, N_2, O_2, CH_4, CO_2, H_2O, H_2, CO, OH, NO, velocity, line Raman for scalar dissipation rate:

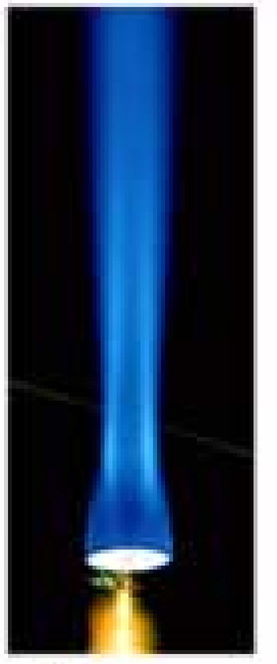
$$\chi = 2\,D\left[\overline{\left(\frac{\partial Z}{\partial x}\right)^2} + \overline{\left(\frac{\partial Z}{\partial y}\right)^2} + \overline{\left(\frac{\partial Z}{\partial z}\right)^2}\right]$$

Lasers for Raman, Rayleigh: Nd:YAG at 532 nm

Lasers for LIF = Nd:YAG + dye: 282 nm for OH, 226 nm For NO, 230 nm for CO (two photon)

Spatial resolution = 0.75 mm

Fluorescence signals were corrected for Boltzmann fraction and collisional quenching rate

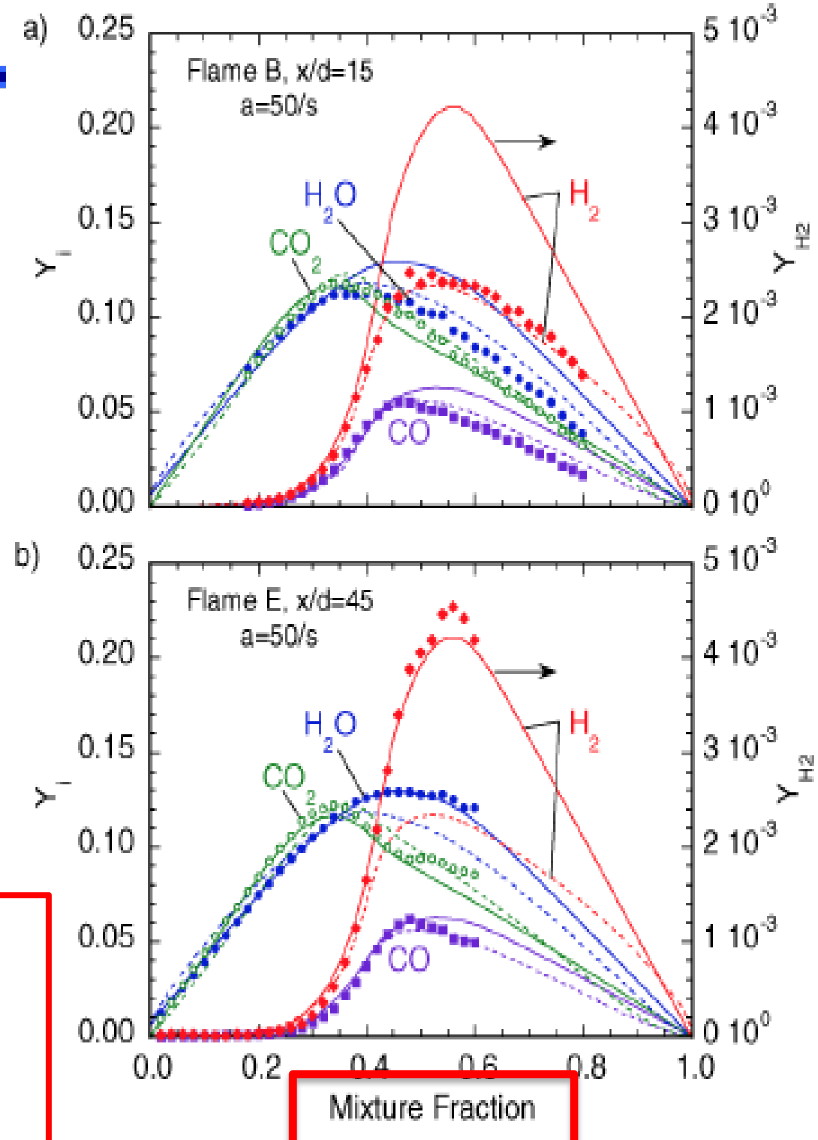


Sandia flame D
Jet diam. = 7.2 mm
Pilot dia = 18.2 mm
Jet U = 50 m/s
Coflow U = 0.9 m/s

Barlow: Non-premixed jet flame

in Comb Flame 143, 433

Fig. 1. Measured conditional means of species mass fractions (symbols) compared with laminar opposed-flow flame calculations including full molecular transport (dashed lines) or equal diffusivities (solid lines). Measurements are shown for (a) flame B at $x/d = 15$ and (b) flame E at $x/d = 45$.



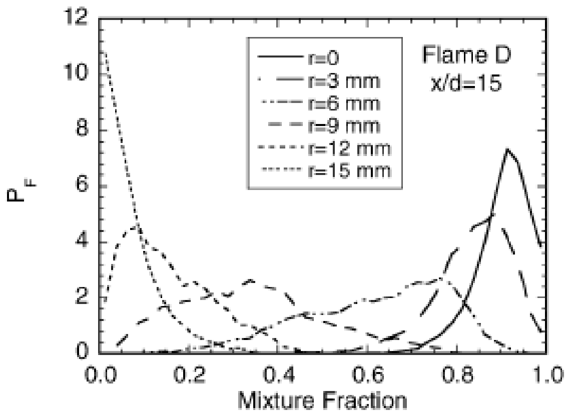
Data points = turbulent jet flame,

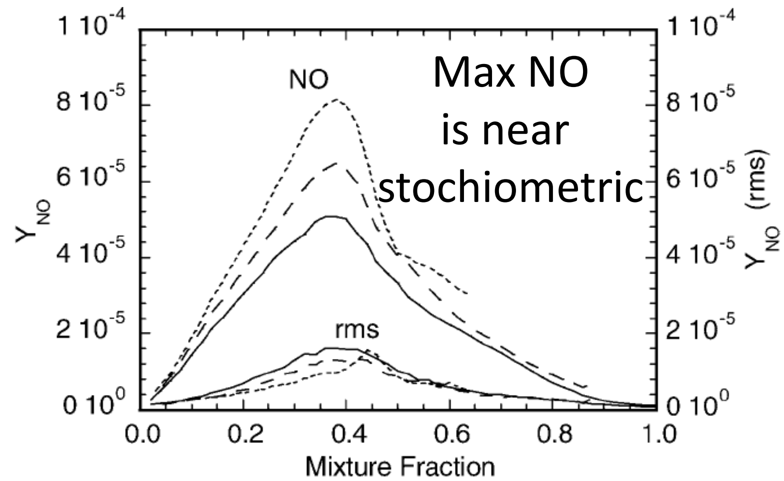
Agree w steady laminar counterflow CHEMKIN = state relations computed for strain parameter $2\ U_{oo}/R = 50\ s^{-1}$

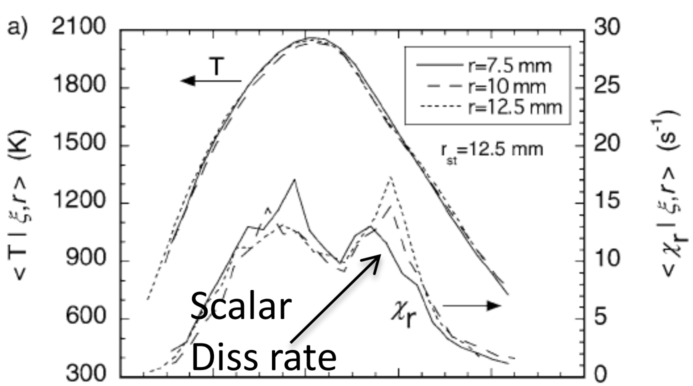
Conclude: steady flamelet state relations
- Adequate for CO & major species
- Not adequate for H_2 or NO
- Differential diffusion is negligible

More Barlow measurements in turbulent non-premixed jet flames

PDF of mixture fraction
is a Beta function





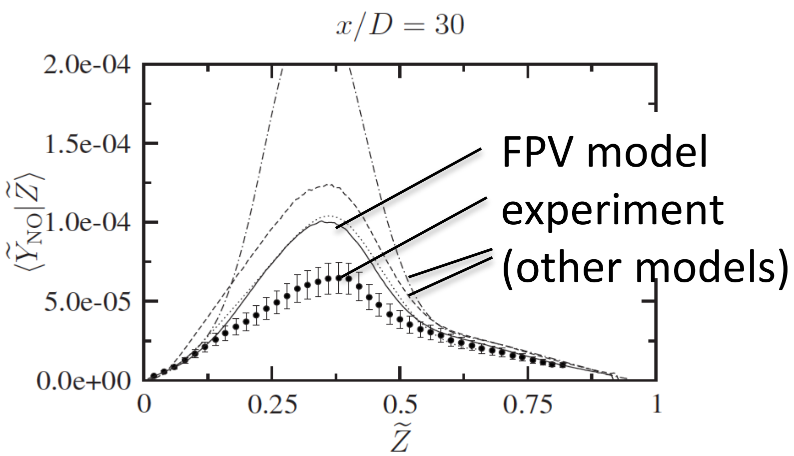


Mixture Fraction

Barlow concludes: all important single point properties were measured in 5 piloted jet non-premixed flames, to be used to assess models

Nitric Oxide - predicted by FPV model compared to non-premixed jet experiment of Barlow

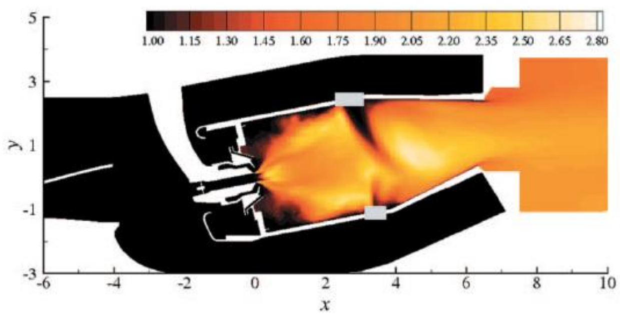
Ihme and Pitsch use FPV to predict NOx in jet flame and in a Pratt gas turbine



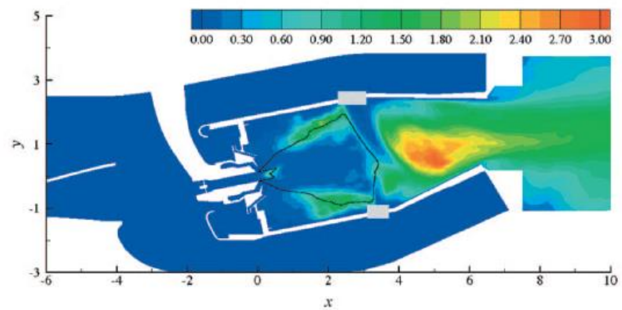
Flamelet progress variable LES overpredicts NO by 40% in a simple jet flame. Not too bad They included radiative heat loss.

Ihme and Pitsch, Modeling of radiation and nitric oxide formation in turbulent non-pre Mixed flames using a flamelet/progress variable formulation, Phys Fluids 20, 055110

NO can be predicted with post-processing (easy)



(c) Averaged temperature (normalized)



(d) Averaged NO mole fraction (normalized)

LES to compute temperature, Y_{N2} and Y_{O2} fields (means and variances)

NO is formed on long time scale so

$$\rho \mathcal{D}_t Y_{\mathrm{NO}} = \nabla \cdot (\rho \alpha \nabla Y_{\mathrm{NO}}) + \rho \dot{\omega}_{\mathrm{NO}}.$$

$O + N_2 \leftarrow\rightarrow NO + N$ etc.

State relation for ω_{NO} obtained from laminar flamelet eqn

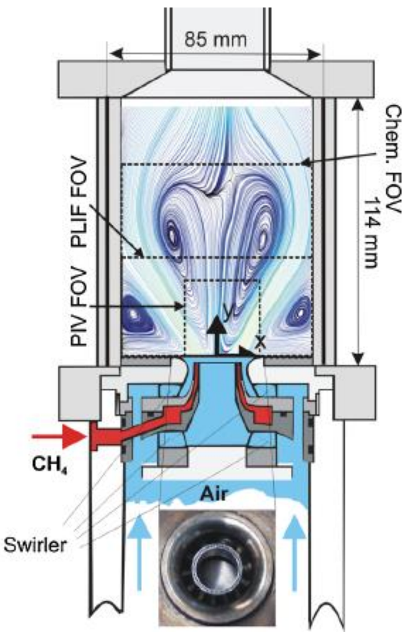
$$\bar{\rho} \widetilde{\mathcal{D}}_t \widetilde{Y}_{\mathrm{NO}} = \nabla \cdot (\bar{\rho} \tilde{\alpha} \nabla \widetilde{Y}_{\mathrm{NO}}) + \nabla \cdot \overline{\boldsymbol{\tau}}_{\mathrm{NO}}^{\mathrm{res}} + \bar{\rho} \tilde{\dot{\omega}}_{\mathrm{NO}},$$

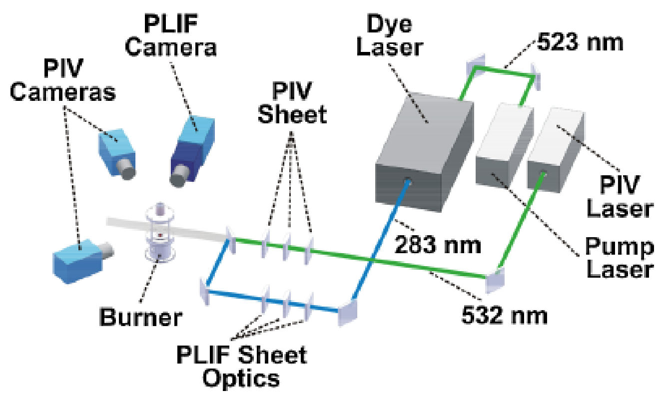
We already know T, Y_O, Y_{N2} from resolved scale LES

Ihme and Pitsch, Modeling of radiation and nitric oxide formation in turbulent non-pre Mixed flames using a flamelet/progress variable formulation, Phys Fluids 20, 055110

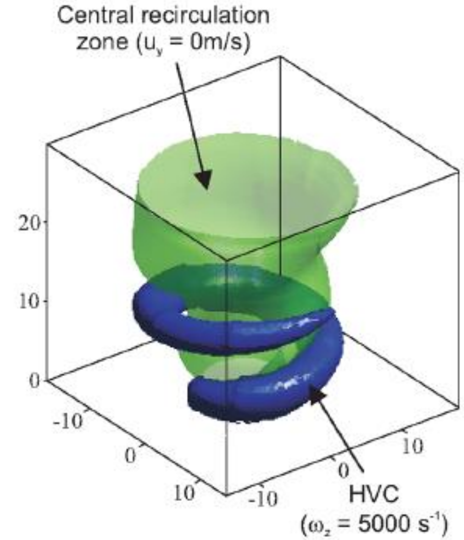
A more complex problem: gas turbine-like swirl flame undergoing unsteady oscillations

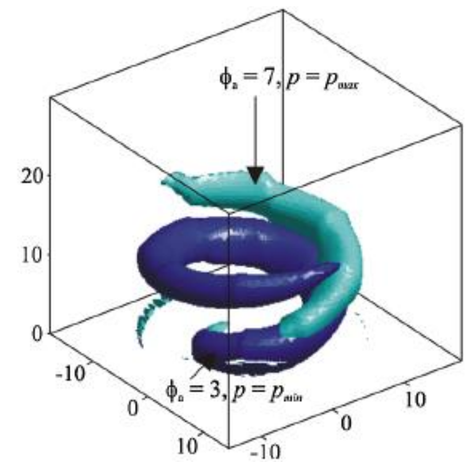
Steinberg, A, , Meier, W. et al., Effects of Flow Structure Dynamics on Thermoacoustic Instabilities in Swirl-Stabilized Combustion, AIAA J. 50, p. 952.

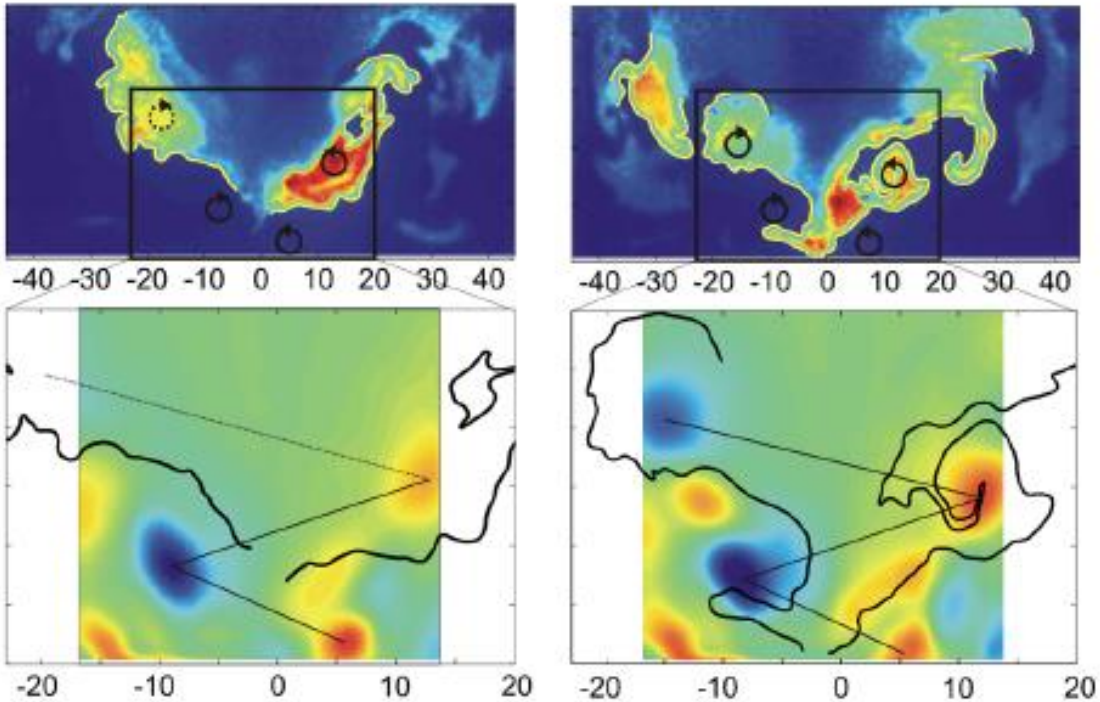




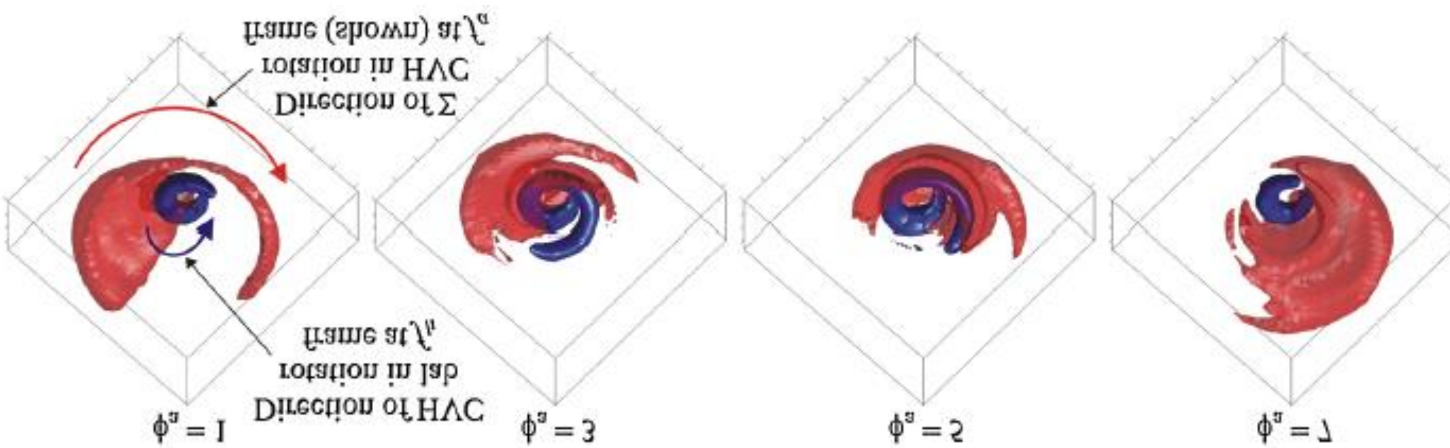
5 kHz PLIF/PIV system







-40 -30 -20 -10 0 10 20 30 40
-40 -30 -20 -10 0 10 20 30 40
-20 -10 0 10 20
-20 -10 0 10 20



Direction of Σ
rotation in HVC
frame (shown) at λ^a
Direction of HVC
rotation in lab
frame at λ^p
ϕ^a = 1
ϕ^a = 3
ϕ^a = 5
ϕ^a = 7

What is the goal of comparing model results to experiments ?

Many models with very different assumptions all “agree” with measurements

Is there any point in comparing output of models without assessing the basic assumptions in the model; i.e., do thin strained flamelets occur in the expt ?

If models agree to within 5%, is there any point to work for better agreement ?

Do we need to include heat losses, complex chemistry, acoustics, pressure ?

Are computations really independent of b.c.s, initial condition, grid size ?

Is the goal to identify the “best” model, or can we live with 20 models ?

How useful are models that do not solve the Navier Stokes eqns ? Some replace NS with Langevin eqn, ad-hoc mixing models, etc. ?

How are we doing ? How well are we making measurements and how well do models compare ?

Review of some good papers - in turbulent combustion

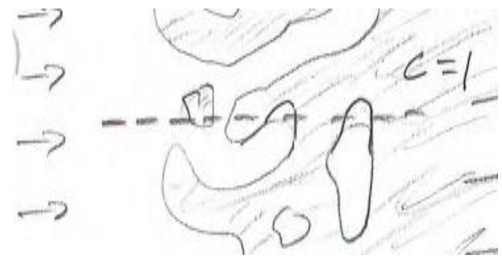
Barlow, R. S., Frank, J. H., A. N. Karpetis, and Chen, J.-Y., "Piloted Methane/Air Jet Flames: Scalar Structure and Transport Effects," Combust. Flame 143:433-449 (2005)

C. Hasse, "LES flamelet-progress variable modeling and measurements of a turbulent partially-premixed dimethyl ether jet flame" Comb Flame 162, 3016

Steinberg, A, , Meier, W. et al., Effects of Flow Structure Dynamics on Thermoacoustic Instabilities in Swirl-Stabilized Combustion, AIAA J. 50, p. 952.

How well can we model premixed turbulent flames ?

Bray / FSD model

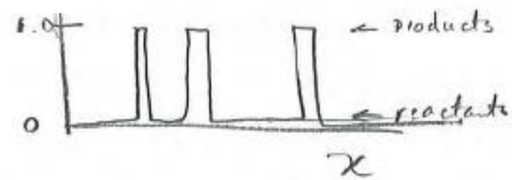


Assume thin or thickened wrinkled flamelets

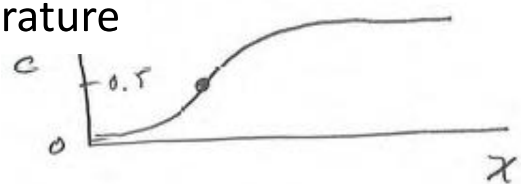
fully premixed or
stratified premixed,
FSD model is being modified
to handle
partially-premixed

considers
corregated (pockets)
flamelet merging
stretch rate increases area

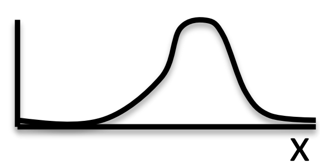
Gas temperature



Mean temperature

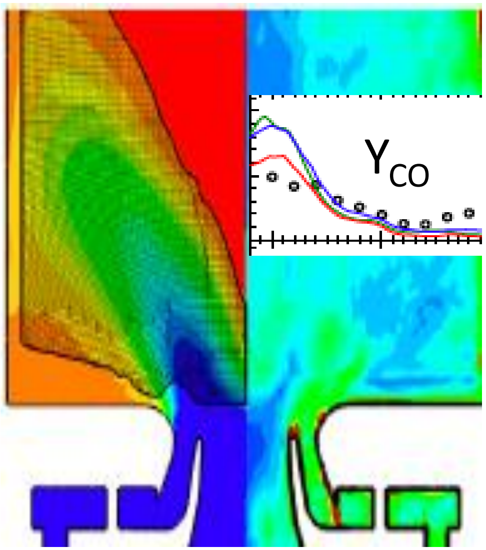


$\Sigma = \mathrm{FSD}$

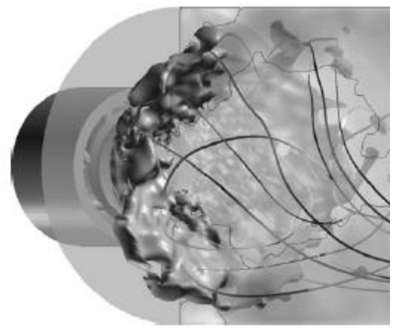


Masuya, Bray, Comb Sci Tech 25, 127

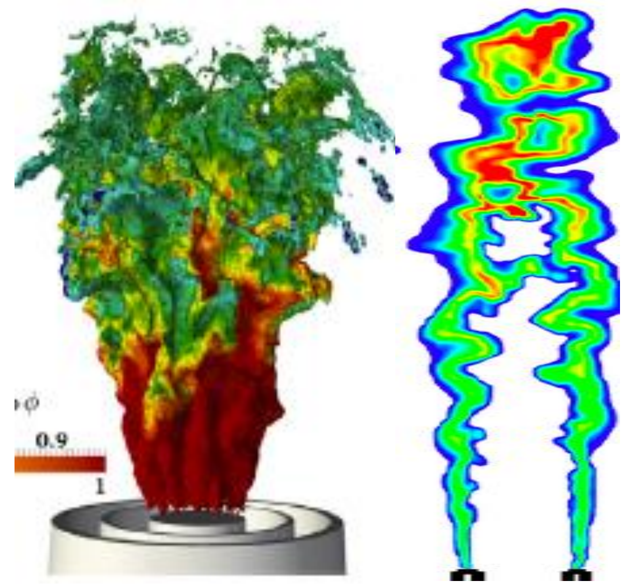
Who is using the Bray / FSD LES method ?



M. Ihme, Stanford U.,
Gas turbine combustor
PROCI 35, 1225



Fureby. Sweden
Gas Turbine Comb.
PROCI 31, 3107



Veynante, Ecole C. Paris
PROCI 35, 1259

Called F-TacLES = Flamelet tabulated chemistry LES

Reactedness = c is the fundamental parameter in premixed turbulent flames

$$c = \frac{T - T_R}{T_P - T_R}$$ = 0 in reactants, =1 in products

Since ρ = p/RT, it follows that inserting the above in for T yields:

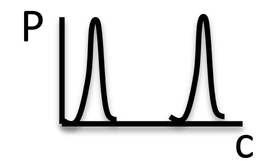
$\boxed{\rho(c) = \rho_R \, (c\,\tau + 1)^{-1}}$ where $\tau = (T_P/T_R - 1)$ = approx. 6 for typical flame

This is called a **state relation** for gas density as a function of c: $\rho(c)$

Probability density function - used to define a mean value

P(c) dc = probability that c lies in the range between c – dc/2 and c + dc/2

$$\bar{\varrho}\ (\bar{c}, \overline{c'^2}) = \int_0^1 \rho(c)\ P(c, \bar{c}, \overline{c'^2})\, dc$$



State relation:

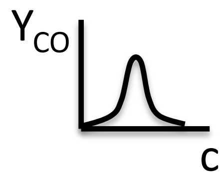
$\rho\,(c) = \rho_R\ (c\,\tau + 1)^{-1}$

At each point in the flame, we solve conservation equations to get the mean $\bar{c}$, and variance $\overline{c'^2}$ and plug into above eqn to get mean density

Idea: you only have to solve conservation equations for $\bar{c}$, and $\overline{c'^2}$ and use above integral to get other mean values; you avoid solving more conservation equations for each variable

Bray / FSD LES model – of premixed turb. flames

State relations - between instantaneous Y_{CO}, ρ, and c from lam. flamelet equation



Assumed shape of PDF(c) of the reactedness (bimodal shape)

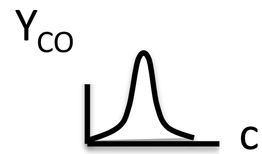
Time averaging

$$\bar{\varrho}\ \left(\bar{c}, \overline{c'^2}\right) = \int_0^1 \rho(c)\ P\left(c, \bar{c}, \overline{c'^2}\right) dc$$

"Lookup tables" between Y_{CO}, T, ρ and c, c'^2

Three conservation equations time-averaged, for
mean reactedness,
variance of reactedness, and FSD (Σ)

State relations - between instantaneous Y_{CO}, ρ, etc. and c from lam. flamelet equation



c = reactedness

Y_P = mass fraction products

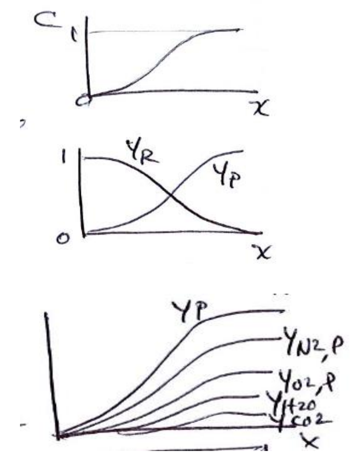
Consider a 1-D, unstretched laminar premixed flame (see text by Law or Kuo, or solve using CHEMKIN)

$$\varrho\, S_L \frac{dc}{dx} = \varrho\, \alpha \frac{d^2 c}{dx^2} + \dot{\omega}_P$$

$$\varrho\, S_L \frac{dY_P}{dx} = \varrho\, \alpha \frac{d^2 Y_P}{dx^2} + \dot{\omega}_P$$

$$\text{thus} \quad c = \frac{T - T_R}{T_P - T_R} = Y_P$$

and $\quad Y_R = 1 - Y_P \quad = 1 - c$



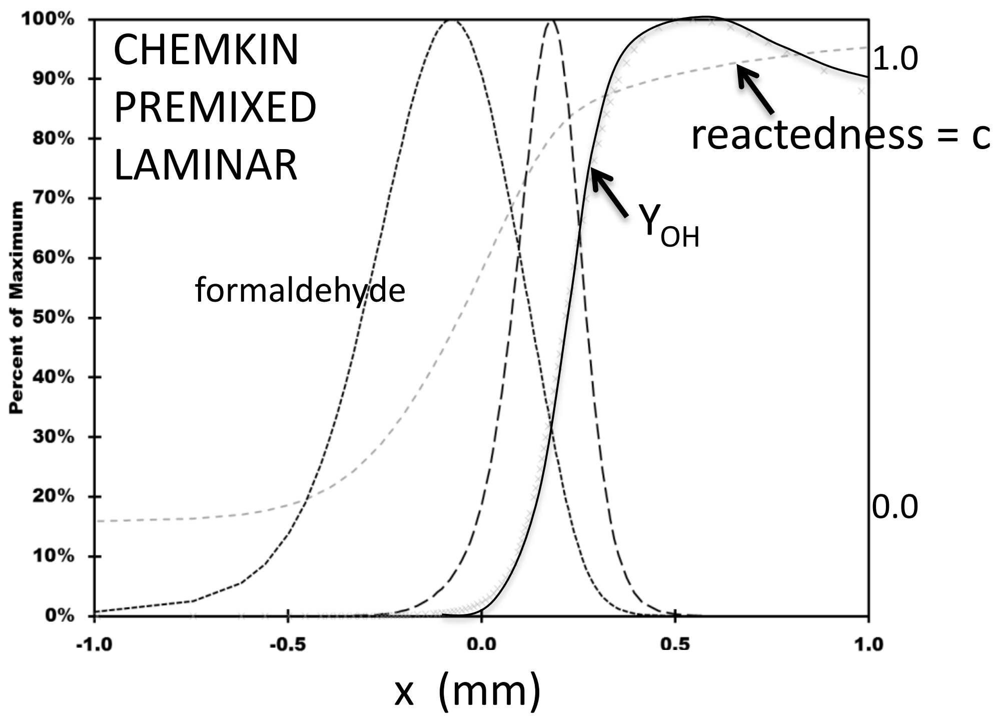
for $CH_4 + 2\, O_2 + 2(79)/21\, N_2 \rightarrow 2\, H_2O + CO_2 + 2(79/21)N_2$

show that $Y_{CH4} = 0.062\, Y_R = 0.062\, (1-c)$ and $Y_{H2O} = 0.12\, Y_P = 0.12\, c$

→ We only have to solve ONE equation (the top one) for c(x) after we represent reaction rate of products $\dot{\omega}_P$ in terms of c and Y_R

→ From *c*(x) we get T(x), ρ(x), Y_R(x), Y_P(x), Y_{CH4}(x), Y_{H2O}(x), etc.

State relations: between Y_i , ρ, T and reactedness c



PREMIXED state relation from CHEMKIN premixed unstrained flamelet

$$\bar{\varrho}\ \left(\bar{c}, \overline{c'^2}\right) = \int_0^1 \rho(c)\ P\left(c, \bar{c}, \overline{c'^2}\right) dc$$

Conservation of mean reactedness

(kg/m^3) (m/s) (1/m) = (kg/m^2/s) (area/vol)

$$\frac{d}{dx}\left(\bar{\rho}\tilde{u}\tilde{c} + \overline{\rho u''c''}\right) = \bar{w} = \rho_R\,(1-c)\,S_L\,\Sigma$$

reaction rate/area

rate of temperature rise in x direction

turbulent flux of temperature fluctuations

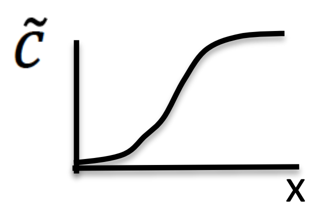
volumetric reaction rate kg/s of products /m^3

Conservation of scalar flux

$$\frac{d}{dx}\left(\bar{\rho}\tilde{u}\frac{\overline{\rho u''c''}}{\bar{\rho}} + \overline{\rho u''^2 c''}\right) + \overline{\rho u''c''}\frac{d\tilde{u}}{dx} + \overline{\rho u''^2}\frac{d\tilde{c}}{dx}$$

$$= -\overline{c''}\frac{d\bar{p}}{dx} + \overline{u''w} - \bar{\chi}_{uc}$$

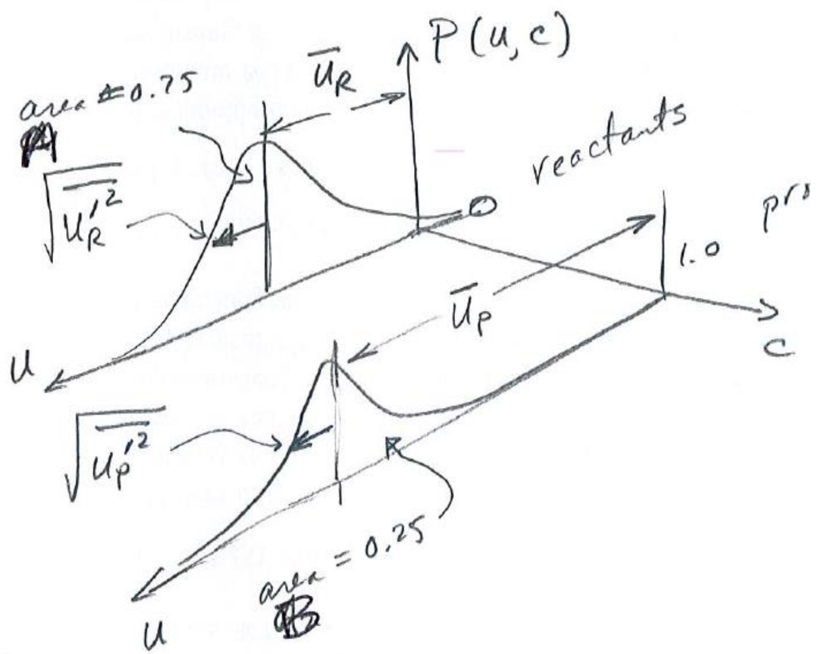
Goal: Two ODEs for the unknowns $\tilde{C}$ and $\overline{\rho u''c''}$



Masuya, Bray, Comb Sci Tech 25, 127, 1981

Bi - Modal PDF for a premixed flame (Bray)

$$P(u,c) = A(u)\,\delta(c) + B(u)\,\delta(1-c)$$



$\delta(c)$ is delta fcn centered at $c = 0$

$\delta(1-c)$ is delta fcn centered at $c = 1$

A(u) and B(u) are Gaussian dist. of velocity

Areas under Gaussians A + B = 1

Mean of A(u) is mean velocity of reactants

Variance of A(u) is variance of reactants

Mean of B(u) is mean velocity of products

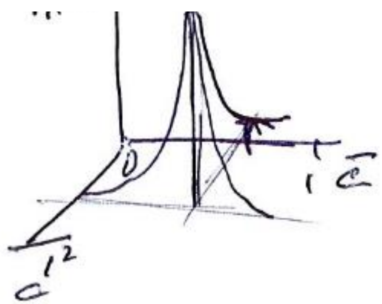
Variance of B(u) is variance of products

"Lookup tables"
between Y_{H2O}, T, ρ
and

$$\left(\bar{c}, \overline{c'^2}\right)$$

$$\overline{Y_{CO2}}\ \left(\bar{c}, \overline{c'^2}\right) = \int_0^1 Y_{CO2}(c)\ P(c, \bar{c}, \overline{c'^2})\, dc$$

$$\overline{Y_{CO2}}\ \left(\bar{c}, \overline{c'^2}\right)$$



Mean CO2 mass fraction depends only on two quantities that are computed at each (x,y,z) location using conservation equations for these two quantities

State relation
Y_{CO2} is a known fraction of Y_P which equals c

Relate all quantities in the two conservation equations to the two unknowns

$\tilde{C}$ and $\overline{\rho u'' c''}$

Bimodal PDF: $P(c) = A\,\delta(c-0) + B\,\delta(c-1)$

example

$$\overline{c'^2} = \overline{(c-\bar{c})^2} = \int_0^1 (c-\bar{c})^2 P(c)\,dc = (c-\bar{c})^2 A\Big|_{c=0} + (c-\bar{c})^2 B\Big|_{c=}$$

$$= \bar{c}^2 A + (1-\bar{c})^2 B$$

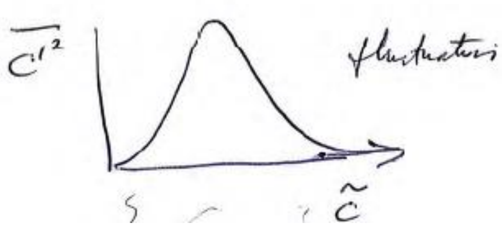
→ plug in $\bar{c}$, A, B formulas which are in terms of $\tilde{c}$

$$= \frac{\tilde{c}^2(\tau+1)^2}{(\tilde{c}\tau+1)^2}\,\frac{(1-\tilde{c})}{(\tilde{c}\tau+1)} + \frac{(\tilde{c})(\tau+1)}{(\tilde{c}\tau+1)}\,\frac{(1-\tilde{c})^2}{(\tilde{c}\tau+1)^2}$$

$$\boxed{\overline{c'^2} = \frac{\tilde{c}(1-\tilde{c})(\tau+1)}{(\tilde{c}\tau+1)^2}}$$

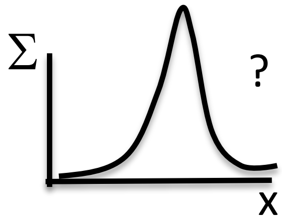
where $\tilde{c}=0$ pure reactants, $\overline{c'^2}=0$

$\tilde{c}=1$ pure products, $\overline{c'^2}=$



There are no fluctuations in reactedness or temperature in the pure reactants or in the pure products

Bray model closure – still have flame surface density Σ (x) in conservation eqn



Σ is proportional to turbulent reaction rate

Third conservation equation must be solved for FSD = Σ

$$\frac{d\,(\tilde{u}\ \Sigma)}{dx} - \frac{d}{dx}\left(\nu_T\ \frac{d\Sigma}{dx}\right) = K\,\Sigma - \mathrm{A}\,\Sigma^2$$

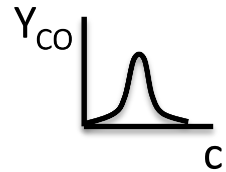
Flame Surface Density Conservation Equation

mean stretch rate K = (u' / L) Γ causes flame area to increase
flamelet merging term A Σ^2 causes flame area to decrease

Final step:
specify correct boundary conditions and solve for $\tilde{u}$ = S_T
= turbulent burning velocity

Bray / FSD LES model – of premixed turb. flames

State relations - between instantaneous Y_{CO}, ρ, and c from lam. flamelet equation



Assumed shape of PDF(c) of the reactedness (bimodal shape)

Time averaging

$$\bar{\rho}\ \left(\bar{c}, \overline{c'^2}\right) = \int_0^1 \rho(c)\ P(c, \bar{c}, \overline{c'^2})\ dc$$

"Lookup tables" between Y_{CO}, T, ρ and c, c'^2

Conservation equations time-averaged, for

mean reactedness
turbulent flux of reactedness
flame surface density (Σ), is prop. to mean reaction rate

Bray / FSD model applied to premixed jet flame

Prasad and Gore
Comb Flame 116,1

Mean Reactedness $\tilde{c}$

$$\frac{\partial \bar{\varrho}\tilde{c}}{\partial t} + \frac{\partial \bar{\varrho}\tilde{u}_k\tilde{c}}{\partial x_k} = \bar{\dot{w}} + \frac{\partial}{\partial x_k}\left(\frac{\mu_t}{\sigma_r}\frac{\partial \tilde{c}}{\partial x_k}\right)$$

Flame Surface Density for Σ

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \tilde{U}_i \Sigma}{\partial x_i} = S_1 + S_2 - D + \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_\Sigma}\frac{\partial \Sigma}{\partial x_i}\right)$$

Axial mom. For $\tilde{u}$

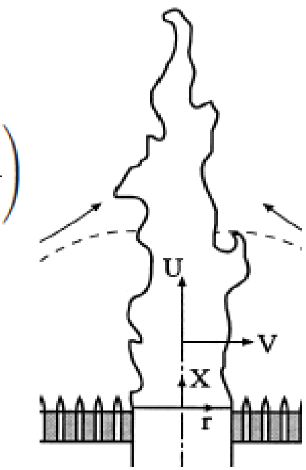
$$\frac{\partial \bar{\varrho}\tilde{u}^2 r}{\partial x} + \frac{\partial \bar{\varrho}\tilde{u}\tilde{v}r}{\partial r} = rg(\varrho_\infty - \bar{\varrho}) + \frac{\partial}{\partial r}\left(r\mu_t\frac{\partial \tilde{u}}{\partial r}\right)$$

Continuity For $\tilde{v}$

$$\frac{\partial \bar{\varrho}\tilde{u}r}{\partial x} + \frac{\partial \bar{\varrho}\tilde{v}r}{\partial r} = 0$$

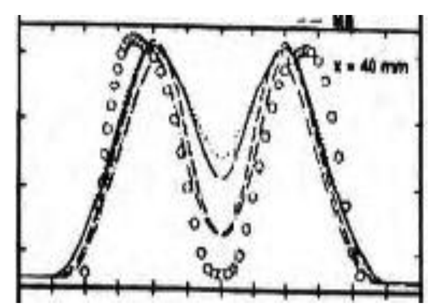
TKE for k, ε

$$\frac{\partial \bar{\varrho}\tilde{u}\tilde{\varphi}r}{\partial x} + \frac{\partial \bar{\varrho}\tilde{v}\tilde{\varphi}r}{\partial r} = rS_\varphi + \frac{\partial}{\partial r}\left(r\frac{\mu_t}{\sigma_\varphi}\frac{\partial \tilde{\varphi}}{\partial r}\right)$$



Mean Temp. (K)

2000
1000
300



r (mm)

Conclude: model predicts correct flame height and turbulent burning velocity (if appropriate constants are selected !)

F-TacLES is Multi-variable approach - for stratified premixed

Filtered TAbulated Chemistry for LES (F-TACLES)

Consider a “stratified” premixed flame - equivalence ratio varies in the reactants

Define Z = mixture fraction = mass fraction of H atoms at a point

Ex. If mixture is $CH_4 + ½\ H_2O$ then Z = 5 / (16 +9) = 0.2

$$\bar{Y}_{CO}\ \left(\bar{c},\overline{c'^2},\bar{Z},\overline{Z'^2}\right)$$
$$= \int_0^1 Y_{CO}(c,Z)\ P_1(c,\bar{c},\overline{c'^2})\ P_2\left(Z,\bar{Z},\overline{Z'^2}\right) dc\, dZ$$

Premixed F-TACLES LES model

"The influence of combustion SGS submodels on the resolved flame propagation. application to the LES of the Cambridge stratified flames"

R. Mercier , T. Schmitt, D. Veynante, B. Fiorina, PROCI 35, 1259

Filtered TAbulated Chemistry for LES (F-TACLES)

model propagates resolved flame at the subgrid scale turbulent flame speed $\mathbf{S_{T,\Delta}}$

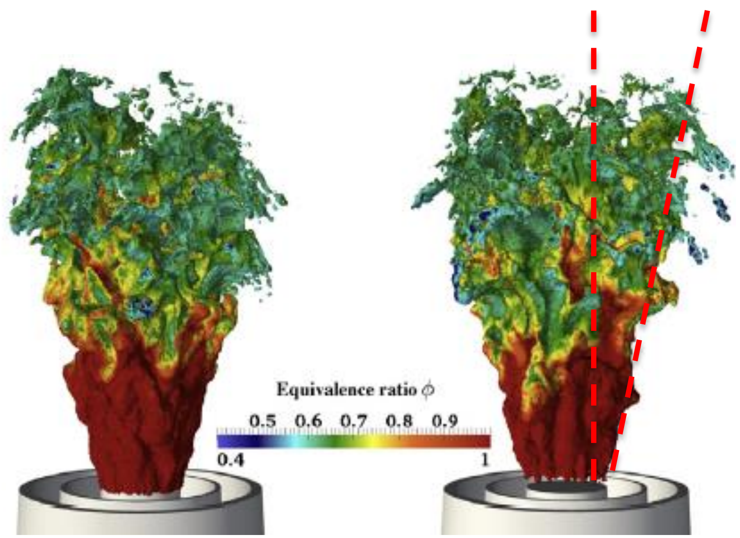
$$\rho_0 S_{T,\Delta} = \Xi_\Delta \gamma \int_0^1 \rho_0 S_l^{ad}(z') P(z')\, dz'$$

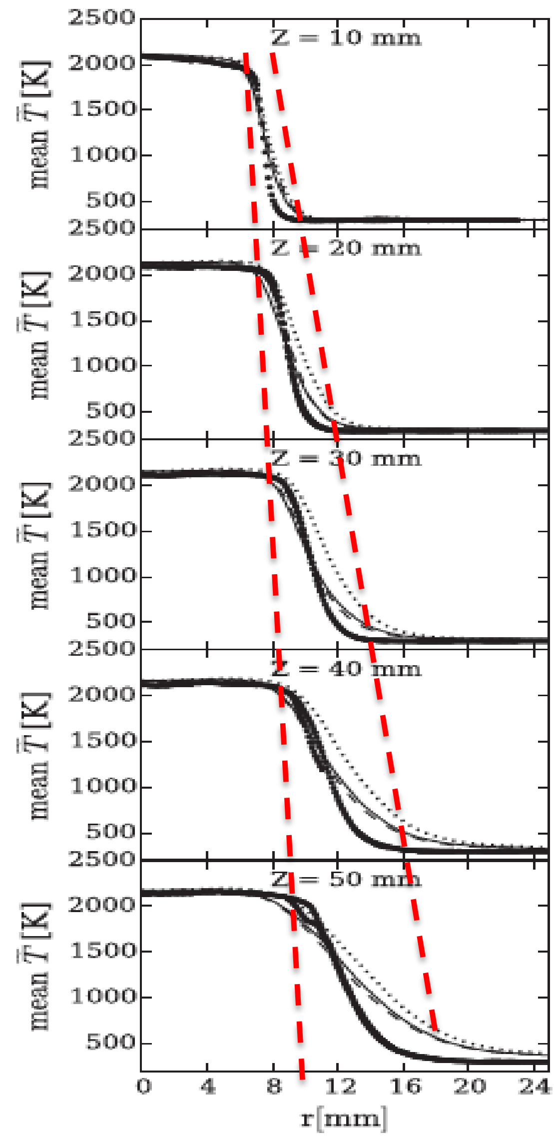
Ξ = new flame surface density parameter

Solves for mean progress variable $\widetilde{Y_c}$

$$\frac{\partial \bar{\rho} \widetilde{Y_c}}{\partial t} + \nabla \cdot (\bar{\rho} \widetilde{\mathbf{u}} \widetilde{Y_c}) = \nabla \cdot \left(\Xi_\Delta \gamma \alpha_{Y_c}^{Tab} \rho_0 D_0 \nabla \widetilde{Y_c} \right) - \Xi_\Delta \gamma \left(\Omega_{Y_c}^{Tab} + \bar{\rho} \widetilde{\dot{\omega}}_{Y_c}^{Tab} \right)$$

Thickness of flame brush computed and agrees with experiment at Cambridge – S. Hochgreb





Flame brush gets wider
As you go upward
Up is plotted down here