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

Eckbreth, Alan, Laser Diagnostics for Combustion Temperature and Species, Combust Science Tech Pub, 1996.

Lockwood, F, Naguib, A, k-epsilon model of jet flame, Comb Flame 24, 109, 1975

Pitsch H, Large-eddy simulation of turbulent combustion, Ann Rev Fluid Mech 38, 2006

Duclos JM, Veynante D, Poinsot T. A comparison of flamelet models for premixed turbulent combustion. Combust Flame 1993; 95: 1 - 16.

Prasad R, Gore JP. Evaluation of flame surface density models for turbulent premixed jet flames. Combust Flame 1999; 116: 1-14.

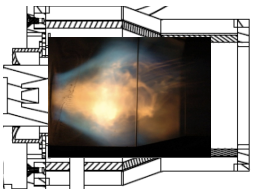
Pitsch, H., LES of turbulent piloted diffusion flame, Phys Fluids 12, 10, 2541, 2000.

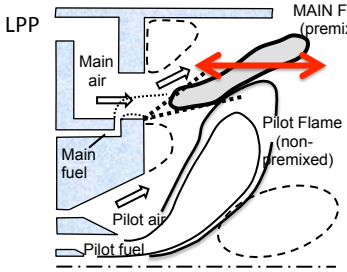
Kalghatgi, G.. Blowout stability limits of gaseous jet diffusion flames in still air, Combust Sci Technol 26, 233, 1981.

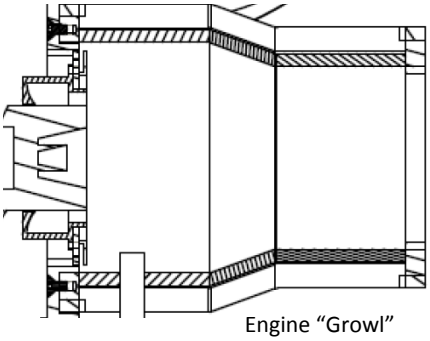
5

Motivation: Premixed is the way of the future - low NOx, CO, soot

GE-TAPS in Michigan High Pressure GT Combustor







Engine "Growl"

premixed flame difficult to anchor
Temme, Driscoll, Combust. Flame 161, 958

Tim Lieuwen – equivalence ratio oscillations
PROCI 27, 1809

6

Motivation - challenges

Most practical problems are "Partially-Premixed"

Partially-Premixed = ER varies in space from 0 to ∞, a point sometimes sees premixed, sometimes non-premixed flamelets

Stratified Premixed = ER varies in space, reactants are within flam. Limits

see: Masri, PROCI 35, 1115, Driscoll Comb Flame 162, 2808

No dependable model of flame blowout, combustion instabilities or turbulent burning velocity at large turbulence level

- Need "robust" LES submodel: **flamelets**: Bray / Flame surface density progress variable (Moin, Pitsch, Ihme)
  thickened: Poinsot (TFM)
  distributed: Menon(LEM), Pope (PDF)
  pyrolysis chemistry (?)

- No measurements of boundaries of regimes - when are flamelet models appropriate ?
- Premixed turbulent combustion is **more difficult** than non-premixed turbulent combustion, not just a mixing problem, also wave propagation

7

Motivation: What problems do we want to solve ?

1. Premixed: Engines: IC engine & HCCI, industrial burners, premixed GT
2. Non-premixed: jet, jet in cross flow, jet in co-flow, jet in swirl flow
3. Partially-premixed: gas turbine, afterburner, base of lifted jet
4. Canonical experiments for model assessment:
   non-premixed: piloted jet flame (Sandia flame D)
   premixed: Bunsen (high-Re), premixed jet, low-swirl, spherical

8

Lewis number effects do not go away at high Reynolds number

Rich hydrogen-air premixed jet flames = very tall, not very wrinkled, have low turbulent burning velocity

Lean hydrogen-air premixed jet flames = short and very wrinkled, have high turbulent burning velocity

For the same laminar burning velocity S_L and same turbulence level u'

Several examples: one is Wu, Driscoll, Faeth, "Preferential Diffusion Effects on the Surface Structure of Turbulent Premixed Hydrogen/Air Flames," Comb. Sci. Technol. 78:69-96, 1991.

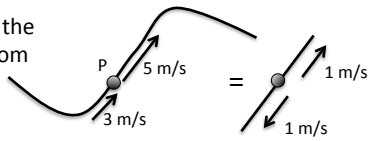
Why does molecular differential diffusion remain important ?

Molecular diffusivity (D) is small compared to turbulent diffusivity (D_T)
But turbulence may not get into reaction layers, so there is no turbulent diffusivity near the reaction region to dominate the molecular diffusivity

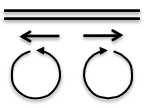
31

Stretched laminar premixed flames (C. K. Law, Princeton)

Near point P in a turbulent premixed flame the tangential velocity of reactants increases from 3 m/s to 5 m/s in the same direction as the tangential velocity, as shown

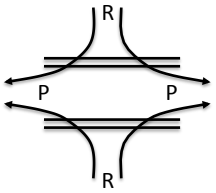


A constant tangential velocity does nothing to the flame equations, so we add a -4 m/s velocity vector to each of these vectors to get the counterflow arrangement on the right



extensive strain from two eddies thins flame

=



Twin counter flow premixed flames

Counterflow is irrotational
Turbulent flow has vorticity

32

Stretch rate of flame surface (K)

$$K = \frac{1}{A}\frac{dA}{dt} = K_s + K_c$$

$= strain + curvature\ components$

$$K_s = -\boldsymbol{n}\cdot(\boldsymbol{n}\cdot\boldsymbol{\nabla})\boldsymbol{V} + \boldsymbol{\nabla}\cdot\boldsymbol{V}$$

$$K_c = \frac{S_L}{R_c}$$

A = flame surface area
n = normal to flame surface pointing toward reactants
V = gas velocity vector
R_c = radius of curvature of flame surface

Example: spherical premixed flame of radius R_f propagating radially outward

$A = 4\pi R_f^2$ so $K = 1/A\ (dA/dt) = (1/(4\pi R_f^2))\ (4\pi)\ (2 R_f\ dR_f/dt) = (2/R_f)\ (dR_f/dt)$

Spherical flame has positive stretch since area is increasing in time

Spherical flame has contributions from both K_s and K_c

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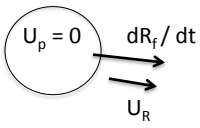
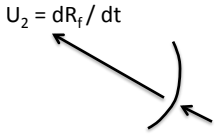
Spherical flame, continued, reactants are pushed radially outward at 200 cm/s

Given: $\rho_1 = 1.2$ kg/m^3, $\rho_2 = 0.2$ kg/m^3
$S_L = 40$ cm/s, and $U_P = 0$

Add a radially inward velocity vector at 240 cm/s to every point



LAB frame of reference



FLAME frame of reference

in flame frame (steady) $\rho_1 U_1 = \rho_2 U_2$ Solve this eqn to find $U_2 = 240$ cm/s
U_2 must equal dR_f/dt and U_1 must equal $dR_f/dt - U_R$

34

Stretched laminar flamelet concept

- Segments of curved premixed laminar flames (such as spherical) and strained turbulent flames are similar to counterflow premixed laminar flames, for the same stretch rate (K) and fuel type. Same for non-premixed too
-

  K = (1/A)(dA/dt)

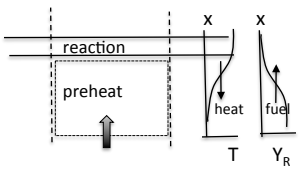
- Stretch rate = has strain rate component, proportional to dV/dy, and a curvature component, proportional to (1/R), R is flame radius of curvature. R is positive for spherically expanding flame, is negative at bunsen tip

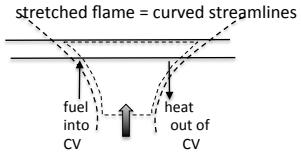
- For a counterflow premixed or non-premixed flame, the velocity gradient (which determines the strain rate) is proportional to the scalar gradient, so the scalar gradient (dissipation rate) often is used instead of the strain rate (velocity gradient)

35

Theory of Flame Stretch C.K. Law Comb Flame 72, 325

Consider a counter flow lean laminar premixed flame – fuel is the deficient reactant





In the unstretched flat flame, heat diffuses upstream, reactants diffuse downstream and nothing leaves through the vertical sides of the control volume, as shown

For the stretched case, streamlines are curved, control volume shape is shown.

Some heat diffuses upstream and out of the control volume, across the curved sides Some reactants diffuse down stream and into the control volume across the curved sides. For every kg/s of fuel that diffuse in about 44,000 kJ/sec of extra heat is added

If more kJ/s of heat diffuses OUT than the kJ/s coming IN with the added reactants, then the flame will propagate slower and extinguish

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Theory of Flame Stretch - Law and Sung

For the stretched flame geometry on last slide, they write balance equations for enthalpy and mass fraction for deficient reactant Y_F (= fuel, assuming fuel-lean) for a hypothetical one step reaction rate: RR = Y_F B exp ($-T_A/T$) where T_A = activation temperature and q_c = heat released per kg fuel

$$(\rho_u S_L A_u)\, c_p\, (T_b - T_u) = \boxed{k \frac{dT}{dx} (A_u - A_b)}^{\text{negative}} + A_b\ q_c \int_{xf}^{xf+} Y_F \,\mathrm{B} \exp\left(-\frac{T_A}{T}\right) dx$$

$$(\rho_u S_L A_u)\, Y_F = \boxed{\rho\, D \frac{dY_F}{dx} (A_u - A_b)}^{\text{positive}} + A_b \int_{xf}^{xf+} Y_F \,\mathrm{B} \exp\left(-\frac{T_A}{T}\right) dx$$

This is similar to the Le Chatlier-Mallard theory for a flat laminar flame, but due to stretch, it now contains different areas A_u and A_b on unburned and burned side
Replace (A_b-A_u) / A_u = Karlovitz number (Ka) = positive for counterflow on last slide

Lewis number Le = (k /$\rho_u c_p$)/D_{def}: if Le >1 heat loss dominates reactant gained → extinction

37

Law's theory of flame stretch correctly predicts burning velocity and burned gas temperature

$$S_L / S_{L,0} = 1 - \mathrm{Ka}\ \mathrm{Ma} \qquad \text{and:}$$

$$T_b = T_{bo} + (T_{b0} - T_u)\,(\mathrm{Le}^{-1} - 1)\ \mathrm{Ka}$$

Ka = nondimensional stretch rate = (stretch rate K) / ($S_{L,02}/\alpha_0$)
= proportional to the velocity gradient
T_b = Burned gas temperature with stretch
Ma = Markstein number for the reactants selected, related to Lewis number
Lean mixtures of light fuels (methane, hydrogen) have Ma <0, Le >1
Lean mixtures of heavy fuels (propane, butane) have Ma>0, Le<1

Conclude:
Bunsen flame tip for lean methane: Ka = negative, Ma=negative>1, Le <1
so stretch causes smaller S_L, lower T_b : we observe an "open tip"
Spherically expanding flame, lean methane: Ka = +, Ma = 1
→so opposite trend; it burns faster

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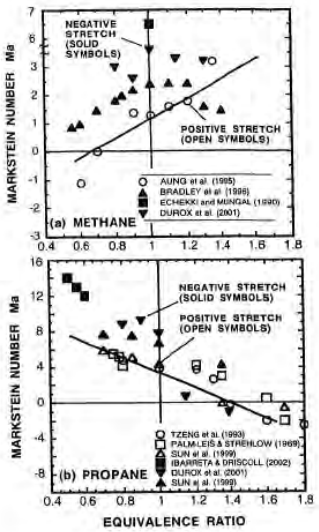


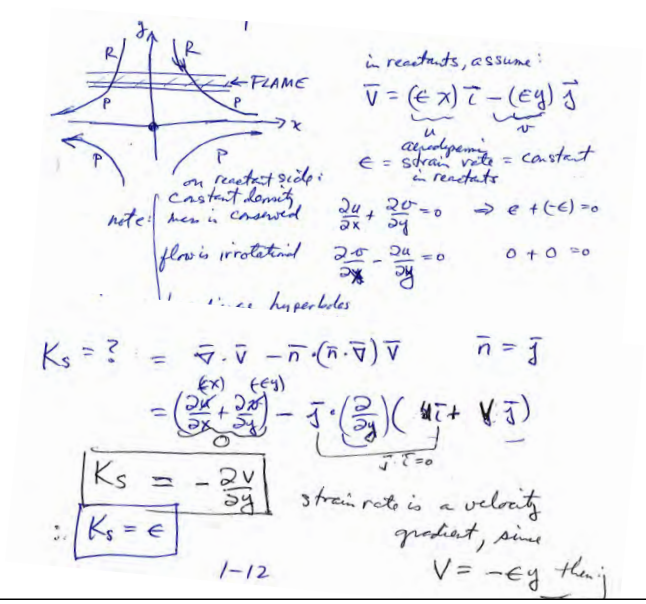
Fig. 1. Markstein numbers measured and computed by previous investigators, showing that larger values of Ma occur for cases of negative stretch. a) methane-air; b) propane-air; reactants at 300 K, 1 atm.

39

End

40

Stretch rate of a counterflow premixed flame



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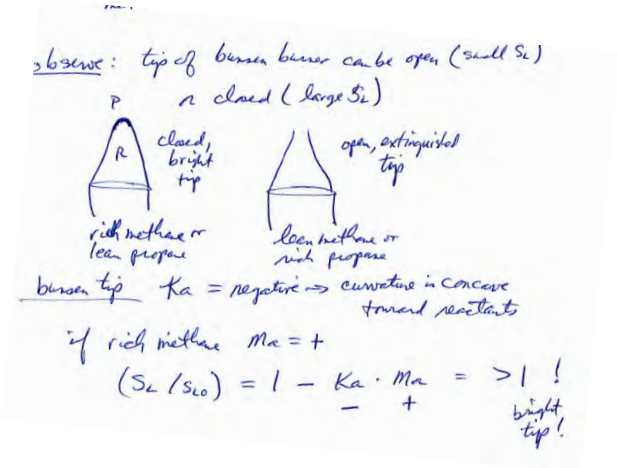
Stretch rate of the tip of a bunsen flame



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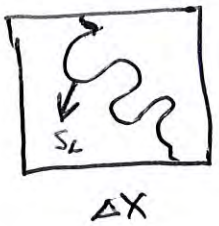
Turbulent Combustion Models - AE 633

NON PREMIXED LES

1	**SLF**	Steady strained laminar flamelet Z eqn with scalar dissipation rate chemistry LES	strained flamelet state relns	Peters, Pitsch
2	**FPV**	Flamelet progress variable Z and c eqns	flamelet state relns	Moin Ihme, Pitsch
3	**PDF**	PDF transport method	parcels	Pope
4	**DNS**	Direct numerical simulation		JH Chen, Ihme

PREMIXED LES			React Rate	authors
1	**FSD**	Flame surface density, also called F-TACLES = tabulated chemistry, Coherent Flamelet Model (CFM)	FSD eqn thin flamelet state relns	Bray, Vervisch Veynante, Fureby Ihme,
2	**FPV**	Flamelet progress variable	thick flamelet	Moin, Ihme Pitsch, Kempf
3	**G Eqn**	G equation	thin flamelet	Pitsch, Bai
4	**TFM**	Thickened flamelet model	thick flamelet	Poinsot
5	**LEM**	Linear eddy model	non flamelet	Menon
6	**DNS**	Direct Numerical Simulation	flamlet, non	Chen, Bell, Aspden



Consider a small volume $(\Delta X)^3$ inside this volume.

$$\bar{\dot{\omega}}_F = \frac{\text{kg/sec fuel consumed}}{\text{volume}} = \text{local reaction rate of fuel at } (x,y,z)$$

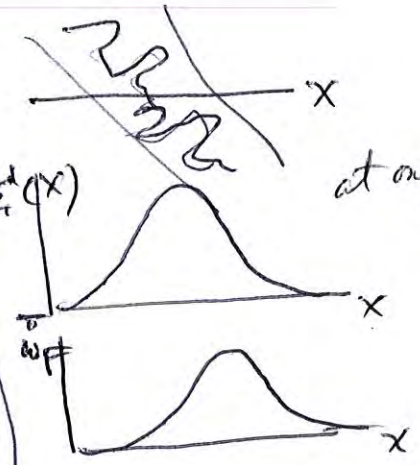
premixed reaction rate (volumetric) = point property

$$\bar{\dot{\omega}}_F = \left(\bar{\rho}\,\bar{Y}_F\right)\left(\bar{S}_L\,\bar{\Sigma}'\right)$$

$\bar{\rho}\,\bar{Y}_F$: $\frac{kg}{vol}$ fuel consumed

$\bar{S}_L$: $\frac{\text{length}}{\text{sec}}$ · $\bar{\Sigma}'$: $\frac{\text{area of flame}}{\text{vol}}$

$\bar{\Sigma}'$ = (vol/sec overtaken by wrinkled surface) / (vol. of box $= \Delta x^3$)



- wrinkled surface has properties of a stretched laminar flame
- turbulence creates large flame area $\bar{A}_f$ → large $\bar{\Sigma}'$
- $\bar{S}_L$ = some averaged laminar burning velocity over wrinkled surface

$$\bar{S}_L = I_0 \cdot S_{L0}$$

$\bar{S}_L$ = stretched laminar burning velocity — averaged over wrinkled surface

S_{L0} = known LBV for reactants

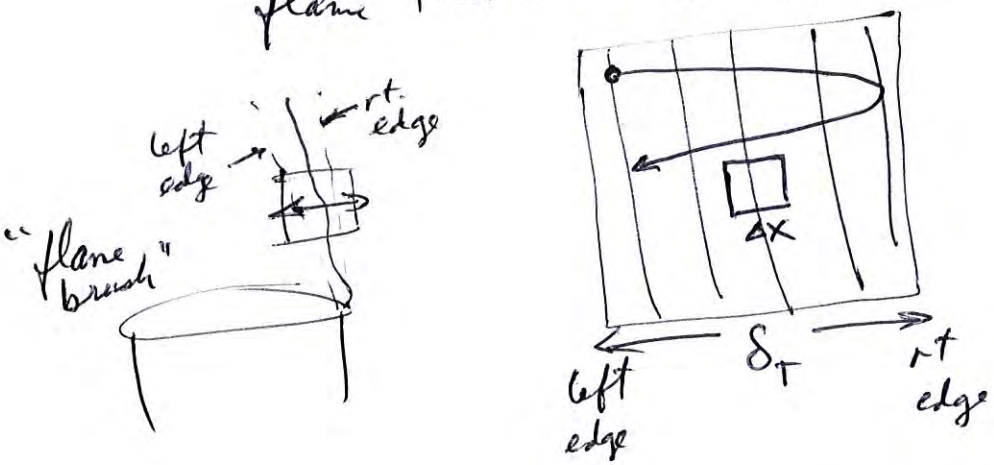
"stretch factor" (to be determined) – depends on Markstein No

$$I_0 = 1 - \bar{K}a \cdot Ma$$

what is Σ physically? dim are cm^{-1}

see Peters p. 51

First Consider an interrogation box in a flat (unwrinkled) flame that is moving left + right



δ_T = brush thickness

put box of size Δx in middle of brush

$$\bar{A}_f = \text{avg area of flame in box} = \underbrace{\left(\text{avg area of flame when it is in box}\right)}_{\Delta x^2} \cdot \left(\text{probability that flame is in box}\right)$$

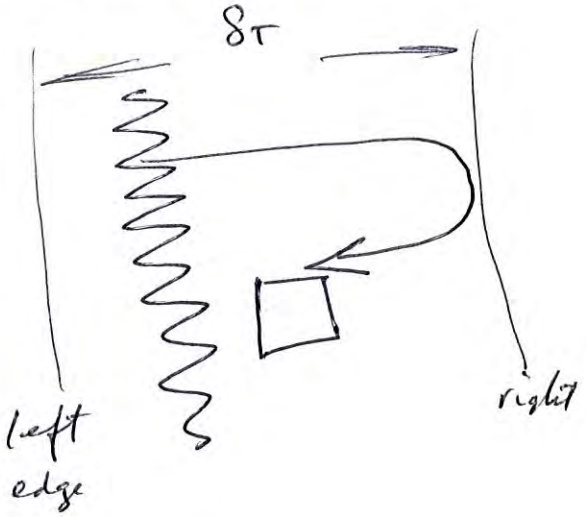
fraction of time flame overlaps box $= \frac{\Delta x}{\delta_T}$

$$\therefore \bar{A}_f = \left(\Delta x^3 / \delta_T\right)$$

$$\text{so } \Sigma = \lim_{\Delta x \to 0} \frac{\bar{A}_f}{\Delta x^3} = \frac{\Delta x^3 / \delta_T}{\Delta x^3} = \frac{1}{\delta_T}$$

real flame is wrinkled!

now consider saw tooth flame oscillating



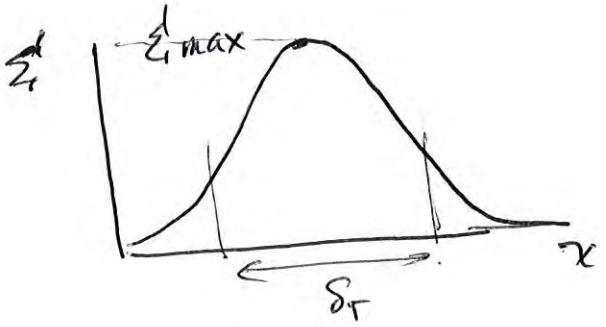
$\frac{A_T}{A_L} = \frac{1}{\sin\alpha}$

A_T = real area in box

$A_L = \Delta x^2$

$$\therefore \quad \Sigma'_{max} \approx \frac{A_T}{A_L} \frac{1}{\delta_T}$$

if we put interrogation box in middle of brush

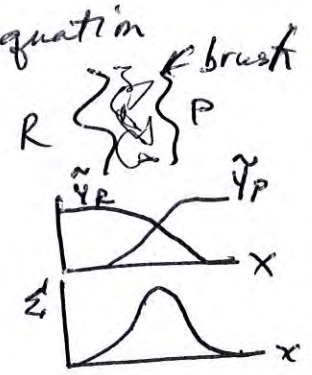


as flame oscillates randomly it infrequently goes past brush boundary — so prob. of flame drops to zero (but not instantaneo

Turbulent reaction rate + Σ' eqn – needed to close the $\tilde{c}$ (reactedness) equation

assume flamelet regime

$$\rightarrow \boxed{\bar{\dot{\omega}}_R = \bar{\rho}\, \tilde{Y}_R\, I_0\, S_{L0}\, \Sigma'}$$



I_0 = stretch factor

Σ' = flame surface density (wrinkling)

need to compute $\Sigma'(x,y,z,t)$ using: see Prasad + Gore

$$\boxed{\frac{\partial \Sigma'}{\partial t} + \frac{\partial}{\partial x_k}\left(\tilde{u}_k \Sigma'\right) = \frac{\partial}{\partial x_k}\left(\frac{\nu_T}{\sigma_\Sigma} \frac{\partial \Sigma'}{\partial x_i}\right) + S_1 + S_2 - D}$$

Σ' = flame surface density (cm^{-1}) flame area / volume

CFM = coherent flamelet model is in FLUENT (see HW #3)

Candel CST 70, 1, 1990

Meneveau CNF 86, 311, 1991

Boudier Proc. Comb Inst 24, 503, 1992

Trouve J. Fluid Mech 1993

Prasad + Gore, CNF 116, 1, 1999

Duclos CNF 95, 101, 1993

σ_Σ = Schmidt number ≈ 0.7

Source terms in Σ' eqn – due to flame stretch (K)

S_1 = rate creation of Σ' from mean flow velocity gradients

S_2 = " turbulent fluctuations

D = destruction flamelet merging

S_1 idea flame area is created by stretch rate (K)

$$K \equiv \frac{1}{A}\frac{dA}{dt}$$ definition of stretch rate K, A = flame wrinkled area

so $$\frac{dA}{dt} = K \cdot A$$

divide by V, take time avg.

$$\frac{d\overline{(A/V)}}{dt} = \overline{K\left(\frac{A}{V}\right)} \Rightarrow \frac{d\Sigma'}{dt} = \underbrace{\overline{K\Sigma'}}_{\text{source terms } S_1 + S_2} \quad (a)$$

(b) $K \approx \frac{\partial \bar{u}}{\partial x} + \frac{\partial u'}{\partial x}$ velocity gradients, but $\frac{\partial u'}{\partial x} \sim \frac{u'_{rms}}{\ell}$ (c)

plug b+c in a

$$\frac{d\Sigma'}{dt} = \underbrace{\frac{d\bar{u}}{dx}\Sigma'}_{S_1} + \underbrace{\overline{\frac{u'}{\ell}\Sigma'}}_{S_2}$$

source terms

$S_1 \sim$ mean velocity gradient

$S_2 \sim$ turbulence velocity fluctuations / integral scale

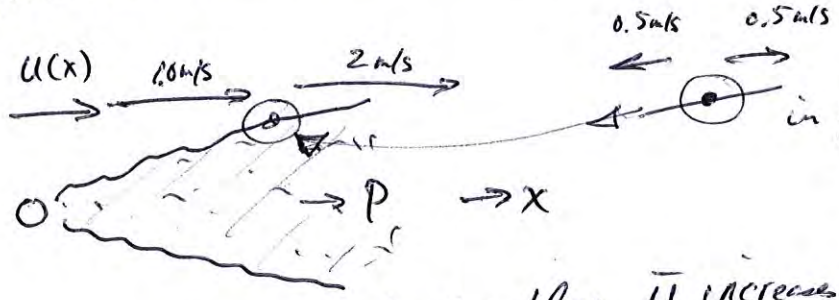
S_1 = rate of production of ξ' due to mean flow velocity gradients (not eddies)

$$S_1 = A_{ik} \frac{\partial \tilde{u}_k}{\partial x_i} \xi'$$

see Prasad + Gore, handout
Dudos 24th symp.
closed: S_1 is in terms of $\bar{u}_k + \xi'$

A_{ik} = flame orientation matrix - from expt. = adjustable!

ex.



rod stabilized flame in accelerating flow $\bar{u}$ increases in x

$$\frac{\partial \bar{u}}{\partial x} = + \qquad A_{11} = 1 \Rightarrow S_1 = \frac{\partial \bar{u}}{\partial x} \xi'$$

flame is stretched by mean flow — (not considering eddies here)

S_2 = rate of production of ξ' due to eddies = velocity fluctuations

$$= \text{const.} \left(\overline{\frac{\partial u'}{\partial x} \xi'} \right) \sim \frac{u'_{rms}}{\ell} \xi'$$

but we said $\frac{u'_{rms}}{\ell} = \frac{\epsilon}{k}$ from production rate = dissipation rate

so

$$S_2 = T_K \frac{\epsilon}{k} \xi'$$

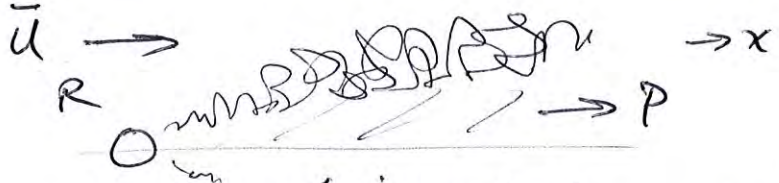
T_K = stretch efficiency function (from DNS, modeling or expt)

closed S_2 is in terms of $\epsilon/k, \xi'$

D = rate of destruction of Σ (flame surface area/vol)

due to flamelet merging

– not due to extinction caused by strain, which heavily depends on chemistry, Ma, etc. – neglect



→ Σ increases in x

production of $\Sigma \sim K\Sigma$ increases in x

Σ cannot grow to ∞, destruction of Σ must occur

merging of flamelets reduces Σ

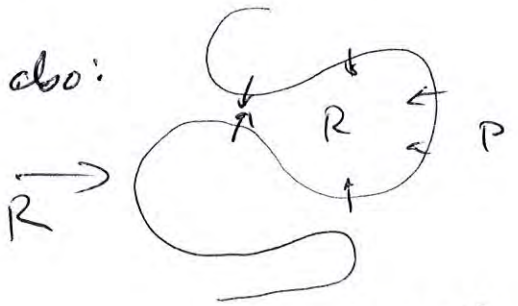
Huygen's principle:

sinusoidal wrinkle

flame burns normal to itself – must form cusps that point to products

cusps burn through destroy area

also:



segments as flames get close to each other – pockets form + burn through

– premixed flame cannot become "fractal" – ∞ wrinkled

assume rate of flame segment "merging" $\sim \Sigma'^2$

analogous to "collisions" in kinetic theory

$$\frac{\text{molecular collisions}}{\text{sec}} \sim \left(\text{number density of molecules}\right)^2$$

in Arrhenius relation

twice the number density $\rightarrow$ 4 × the collisions/sec

$$D = \frac{\text{loss of } \Sigma'}{\text{time}} = \mathbb{B}\cdot \Sigma'^2 = (\Sigma'/\text{sec})\,\Sigma' = cm^{-1} = cm^{-1}s^{-1}$$

$$\frac{(\Sigma'/t)}{\Sigma'^2} = \frac{cm^{-1}s^{-1}}{(cm^{-1})^2} = \frac{cm}{sec} = \text{speed}$$

$\mathbb{B}$ must have dimensions of

two speeds are relevant $S_{L0} + k^{1/2}$

speculate $\mathbb{B} \sim \left(S_{L0} + c_1 k^{1/2}\right) \sim \frac{m}{sec}$

by dimensional reasoning — these are the only two velocities of importance: $\bar{u}$ is not

ie larger S_{L0} $\rightarrow$ flamelet merge faster

larger $u' \sim k^{1/2}$ "

$$\boxed{D = \text{const.}\left(S_{L0} + c_1 k^{1/2}\right)\Sigma'^2}$$

destruction rate

in coherent flamelet model see Prasad + Gore handout

Coherent Flamelet Model (CFM)

An Evaluation of Flame Surface Density Models for Turbulent Premixed Jet Flames

R. O. S. PRASAD and J. P. GORE*

COMBUSTION AND FLAME 116:1–14 (1999)

CFM = RANS version

FLACLES = LES version

Stoichiometric methane–air jet flame stabilized in a coflow of reactants at the same air–fuel ratio as that of the main jet. A schematic diagram of the burner used in their experiments is shown in Fig. 1. It consists of a 12-mm-diameter central tube through which premixed fuel and air are supplied. The central tube is surrounded by a 68-mm-diameter annulus

a) Continuity equation

for $\tilde{V}$

$$\frac{\partial \bar{\rho}\tilde{u}r}{\partial x} + \frac{\partial \bar{\rho}\tilde{v}r}{\partial r} = 0 \qquad (9)$$

b) Axial momentum equation

for $\tilde{u}$

$$\frac{\partial \bar{\rho}\tilde{u}^2 r}{\partial x} + \frac{\partial \bar{\rho}\tilde{u}\tilde{v}r}{\partial r} = rg(\rho_\infty - \bar{\rho}) + \frac{\partial}{\partial r}\left(r\mu_t \frac{\partial \tilde{u}}{\partial r}\right) \qquad (10)$$

c) Transport equation for turbulent kinetic energy and turbulent dissipation rate

for k, ϵ

$$\frac{\partial \bar{\rho}\tilde{u}\tilde{\varphi}r}{\partial x} + \frac{\partial \bar{\rho}\tilde{v}\tilde{\varphi}r}{\partial r} = rS_\varphi + \frac{\partial}{\partial r}\left(r\frac{\mu_t}{\sigma_\varphi}\frac{\partial \tilde{\varphi}}{\partial r}\right) \qquad (11)$$

Here $\tilde{\varphi} = \tilde{k}$ and $\tilde{\epsilon}$. The source terms and the turbulent Prandtl numbers for these equations are taken as follows:

$$S_k = \mu_t\left(\frac{\partial \tilde{u}}{\partial r}\right)^2 - \bar{\rho}\tilde{\epsilon},\ \sigma_k = 1.0 \qquad (12a)$$

$$S_\epsilon = C_{\epsilon 1}\mu_t\left(\frac{\partial \tilde{u}}{\partial r}\right)^2 - C_{\epsilon 2}\bar{\rho}\frac{\tilde{\epsilon}^2}{\tilde{k}},\ \sigma_\epsilon = 1.3 \qquad (12b)$$

The turbulent viscosity is given by $\mu_t = C_\mu \bar{\rho}\tilde{k}^2/\tilde{\epsilon}$, where $C_\mu = 0.09$, $C_{\epsilon 1} = 1.44$, and $C_{\epsilon 2} = 1.87$. Except for $C_{\epsilon 2}$, all the empirical constants are same as those in the standard k-ϵ model. $C_{\epsilon 2}$ is taken as 1.87 following Jeng and Faeth [31],

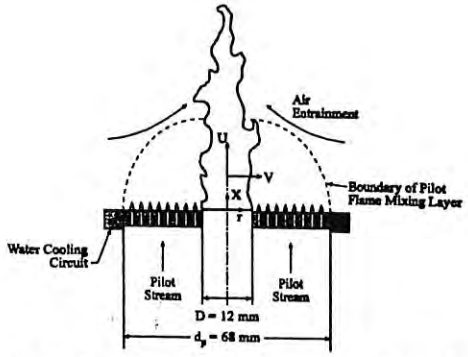


Fig. 1. Schematic diagram of the premixed burner used by Chen et al. [2].

$\bar{\rho}$ → from assumed PDF = two delta functions – in terms of $\tilde{c}$

$\bar{P}$ = constant (assumed)

$\tilde{Y}_R, \tilde{Y}_P, \tilde{Y}_F, \tilde{Y}_i, \tilde{T}, \widetilde{T''^2}$ → from PDF and $\tilde{c}$

for $\tilde{c}$

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

Turbulent reaction rate: $\bar{\dot{\omega}} = \bar{\rho}\tilde{Y}_R S_L \Sigma,$ Reaction Rate

Flame Surface Density Balance Equation

for Σ

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

where source terms are:

$$c = \frac{T - T_R}{T_P - T_R}$$

reacted mass

Surface density balance equation derived in:

23. Pope, S. B., *Int. J. Engng Sci.* 26:445–469 (1988).
24. Candel, S. M., and Poinsot, T., *Combust. Sci. Technol.* 70:1–15 (1990).

TABLE 1

Production and Destruction Terms in Flame Surface Density Models

Model	S_1	S_2	D
CPB	$A_{ik}\frac{\partial \tilde{U}_k}{\partial x_i}\Sigma$	$\alpha_o C_A(\epsilon/\nu)^{1/2}\,\Sigma$	$\alpha_o S_L \frac{2+e^{-aR}}{3\left(\frac{Y_F}{Y_{Fo}}\right)}\Sigma^2$
		$\alpha_o = 1.$ $C_A = 0.28$	$\alpha_o = 1.0$, a = 10,
			$R = \frac{Y\epsilon}{Y_o \Sigma S_L k}$
CFM	$A_{ik}\frac{\partial \tilde{U}_k}{\partial x_i}\Sigma$	$\alpha_o \frac{\epsilon}{k}\Sigma$	$\beta_o \frac{S_L + Ck^{1/2}}{\frac{Y_F}{Y_{Fo}}}\Sigma^2$
		$\alpha_o = 1.7$	$\beta_o = 1$, C = 0.5
MB	$E\frac{u_i^1 u_j^1}{k}\frac{\partial \tilde{U}_k}{\partial x_i}\Sigma$	$\alpha_o Re_t^{1/2}\frac{\epsilon}{k}\Sigma$	$\frac{\beta_o S_L Re_t^{1/2}}{\frac{Y_F}{Y_{Fo}}\left(1-\frac{Y_F}{Y_{Fo}}\right)\left(1+c\frac{S_L}{k^{1/2}}\right)^{2\gamma}}\Sigma^2$
	E = 0.5	$\alpha_o = 0.9$	$\beta_o = 1.25$, c = 1, $\gamma = 0.5$
CD		$\alpha_o \lambda \frac{\epsilon}{k}\Sigma$	$\beta_o \frac{S_L}{\frac{Y_F}{R_{Fo}}}\Sigma^2$
		if $k_t \le \alpha_o K \frac{S_L}{\delta_L}$	$\beta_o = 5.0$
		$\alpha_o = 5.0$, λ =8.5, K = 10	

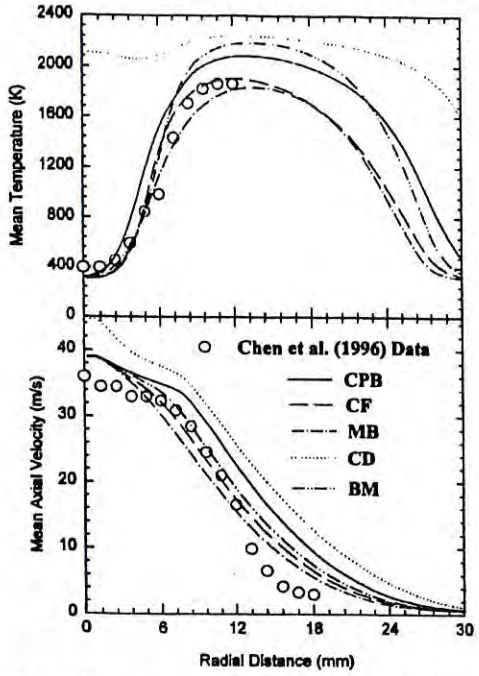


Fig. 4. Predictions of mean temperature and axial velocity at $x/D = 6.5$.

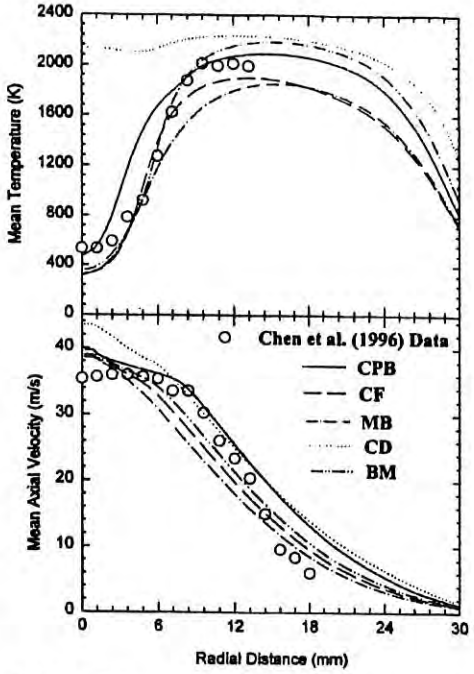
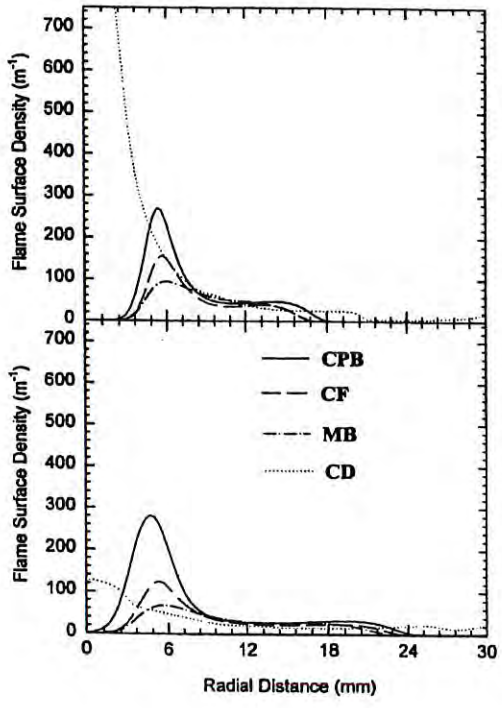
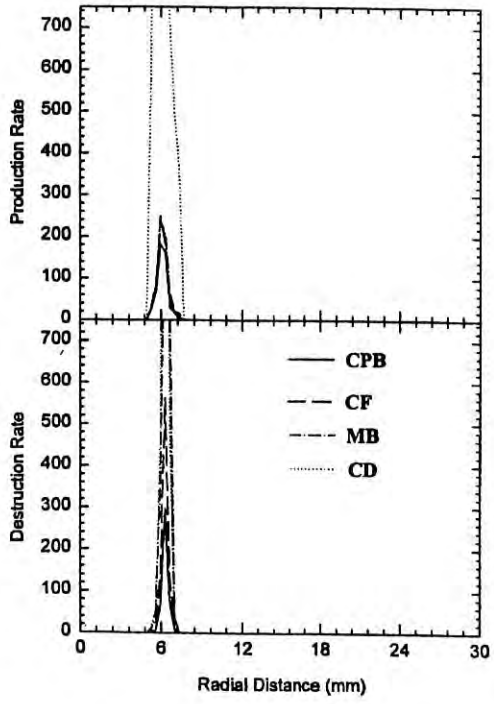


Fig. 5. Predictions of mean temperature and axial velocity at $x/D = 8.5$.





Also:

An evaluation of combined flame surface density and mixture fraction models for nonisenthalpic premixed turbulent flames • ARTICLE
Combustion and Flame, Volume 117, Issue 3, May 1999, Pages 514-528
R. O. S. Prasad, R. N. Paul, Y. R. Sivathanu and J. P. Gore

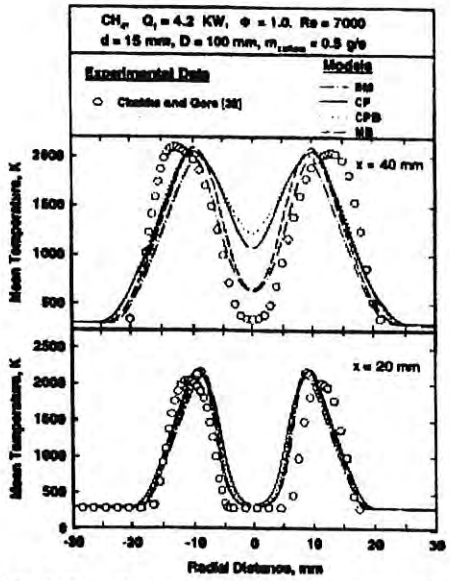


Fig. 4. Comparisons of mean temperature between different model predictions and experimental data for axial locations x = 20 mm and 40 mm respectively.

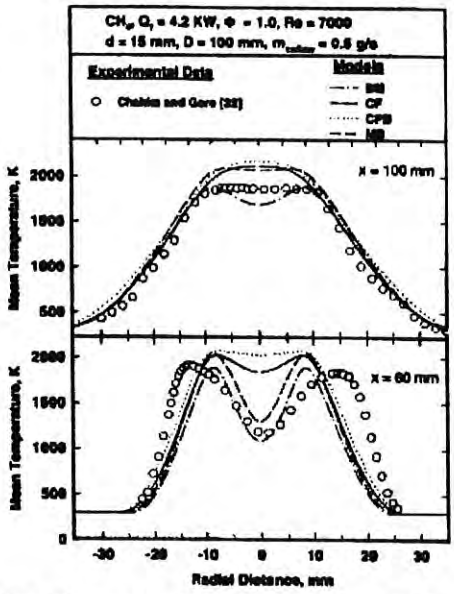
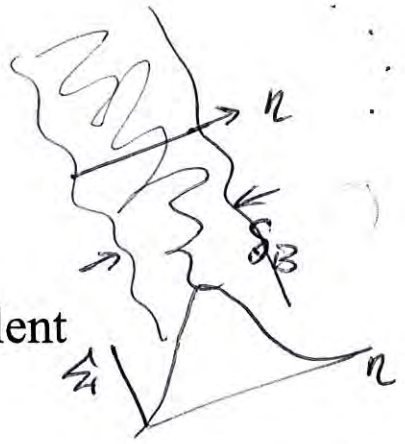


Fig. 5. Comparisons of mean temperature between different model predictions and experimental data for axial locations x = 60 mm and 100 mm respectively.

CFM predicts mean temperature profiles for a Bunsen flame that agree with experiment

Flame height is correctly predicted – note two peaks merge at x = 100 mm – at tip of Bunsen flame. Therefore turbulent burning velocity is correctly predicted.

Coherent Flamelet Model: Computed Flame Surface Density and Turbulent Burning Velocity



$$\frac{S_T}{S_{L0}} = I_0 \int_{-\infty}^{\infty} \Sigma \, d\eta$$

$\frac{S_T}{S_{L0}} = \frac{A_T}{A_L}$

$= \underbrace{\text{wrinkled area/volume}}_{\bar{\Sigma}_1} \cdot \underbrace{\frac{(\text{volume})}{A_L}}_{\text{brush thickness}}$

$= \bar{\Sigma}_1 \, \delta_B$

where $\bar{\Sigma}_1 = \frac{\int \Sigma_1' \, d\eta}{\delta_B}$

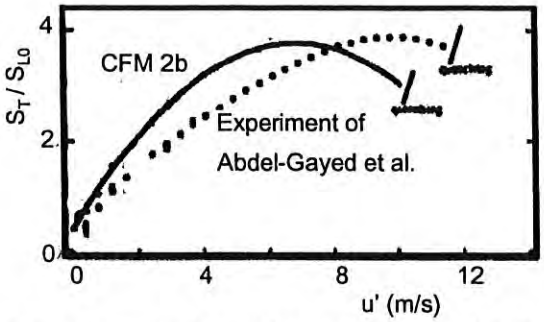


Figure 31. Results of Duclos et al. [24] showing that the Coherent Flamelet Model can predict the turbulent burning velocity data of Abdel-Gayed et al. [43]. Note that CFM predicts the correct "bending" of this curve that is caused by the loss of flame surface area due to flamelet merging and quenching at large turbulence intensities. The model simulates a planar turbulent flame having one dimensional mean properties.

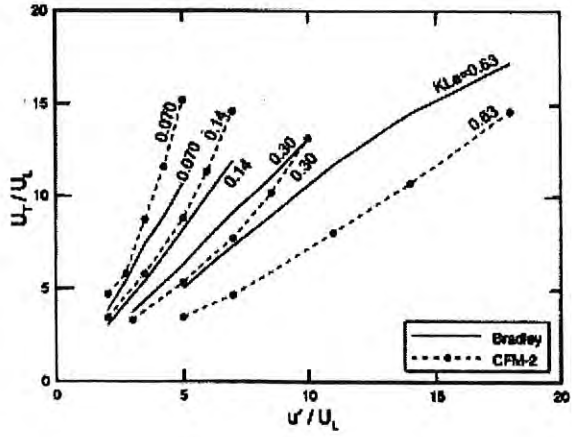


Figure 32. Comparison of Turbulent Burning Velocity Predicted by the Coherent Flamelet Model of Choi and Huh [28] to the Measurements of Bradley [42]. The model considers a spherical expanding turbulent flame in a chamber.

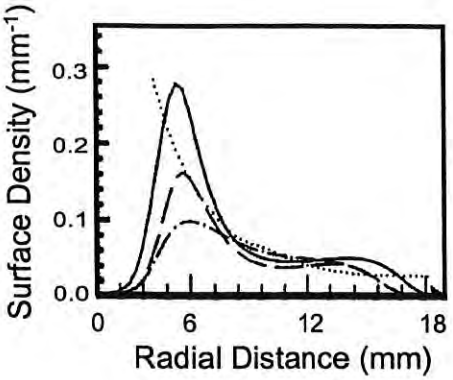


Figure 22. Computed profiles of surface density for a Bunsen flame; the Coherent Flamelet Model was used by Prasad and Gore [26]. The three curves correspond to different models used to determine the source term in the equation for flame surface density.

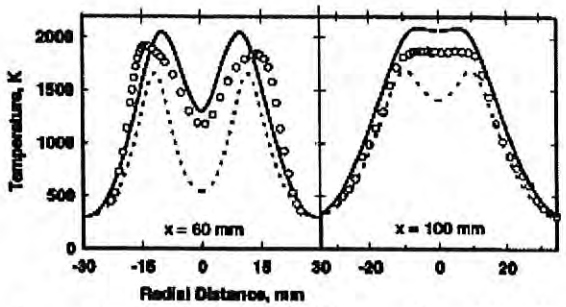


Figure 33. (a) Comparison of temperature profiles predicted by the Coherent Flamelet Model of Prasad and Gore [26] to thermocouple measurements made in an identical turbulent Bunsen flame. The agreement indicates that the model is predicting a realistic flame height (where the temperature profile is no longer bimodal) and a realistic turbulent burning velocity. (b) Flame surface density across the brush of the Bunsen flame computed by Prasad and Gore.

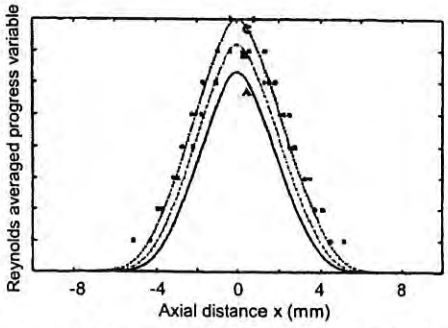


Figure 34. Comparison of mean reactedness computed by the Coherent Flamelet Model of Wu and Bray (solid and dashed lines) to the measured values of Kostiuk[12]. CFM predicts a realistic location of the flame within the counterflow velocity field, indicating that the predicted turbulent burning velocity is in agreement with the experiment.

How to compute $\bar{\rho}$, $\bar{T}$, $\bar{Y}_{H2O}$ etc?

need state relations $\rho = \rho(c)$

need $P(c)$ $T = T(c)$

$Y_{H2O} = Y_{H2O}(c)$

plug into

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

$$\bar{T} = \int_0^1 T(c)\, P(c)\, dc$$

$$\bar{Y}_{H2O} = \int_0^1 Y_{H2O}(c)\, P(c)\, dc$$

Need the PDF (c) – for Prasad-Gore CFM model

– he solves $\tilde{c}$ eqn for $\tilde{c}$ = nondim. temperature = reactedness = 0 reactants, 1 products

we need P(c) to determine: $\bar{\rho}$, $\bar{Y}_{H_2}$, $\tilde{T}$

state relation $\rho = \frac{P}{R} T^{-1}$ $\quad c = \frac{T - T_R}{T_P - T_R}$ $\quad \therefore T = c(T_P - T_R) + T_R$

define: $\tau = (T_P/T_R - 1) \approx \frac{2100}{300} - 1 = 6$

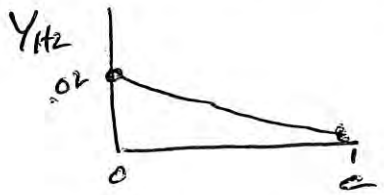
combine (a) $\boxed{\rho(c) = \rho_R (c\tau + 1)^{-1}}$ state relation for $\rho(c)$

so $\bar{\rho} = \rho_R \int_0^1 (c\tau+1)^{-1} P(c)\, dc$ → we need $\tilde{c}$, $\widetilde{T^2}$ shape of P(c)

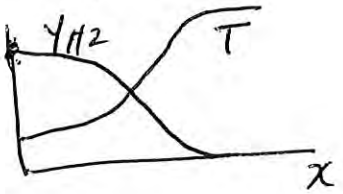
similarly (b) $\boxed{\bar{Y}_{H_2} = \int_0^1 Y_{H_2}(c)\, P(c)\, dc}$

suppose $Y_{H_2} = 0.02$ in reactants ($c=0$) (Stoich H_2-air $Y_{H_2} = .029$)

$Y_{H_2} = 0$ in products $c=1$

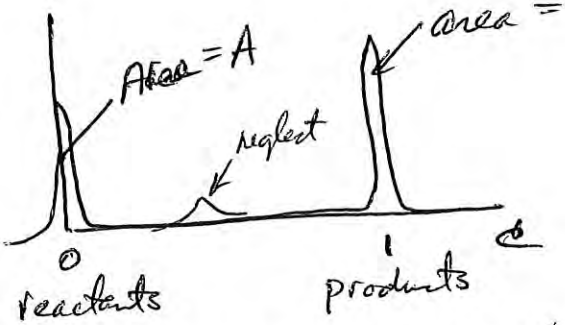


get this curve from laminar flamelet solution cross plot these 2 curves for zero strain rate equil chemistry:



Bray: assume $P(c)$ is a <u>double delta function</u>

$P(c) =$



$A + B = 1$

assume very thin flamelets so probability finding $c = 0.5$ (partially burned) is very small, ignore

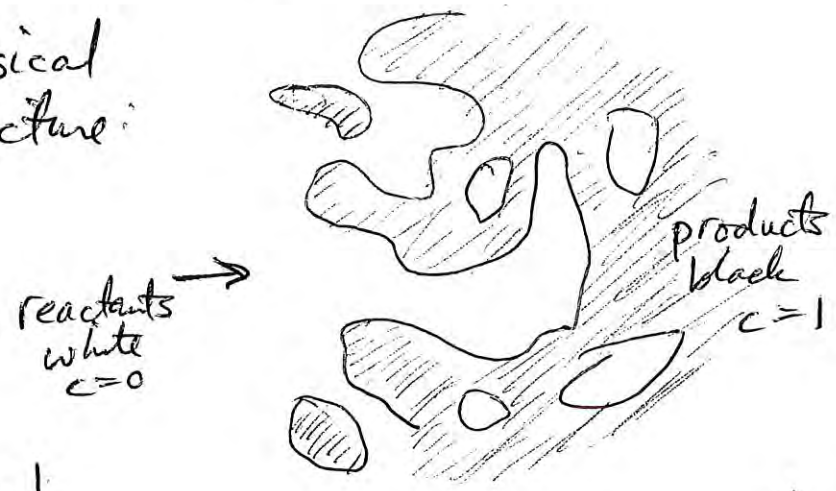
$$\boxed{P(c) = A\,\delta(c-0) + B\,\delta(c-1)}$$

δ = delta fcn $\qquad \int_0^1 \delta(0)\,dc = 1$

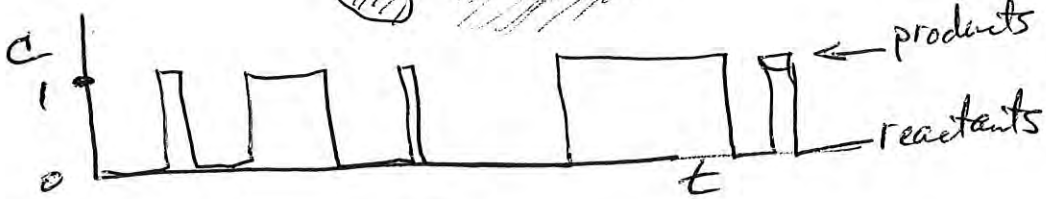
$$\int_0^1 P(c)\,dc = A\int \delta(0-0)\Big|_{c=0}^{1} dc + B\int \delta(1-1)\Big|_{c=1}^{1} dc$$

$$= A + B = 1$$

physical picture:



this yields a PDF with double delta function



$$\tilde{c} = \frac{\overline{\rho c}}{\bar{\rho}} = \frac{\int_0^1 \rho \cdot c \; P(c)\,dc}{\bar{\rho}} = \frac{\int_0^1 \left(\frac{c}{(c\tau+1)}\right)\left(A\,\delta(0) + B\,\delta(1)\right)dc}{\left(A + B(\tau+1)^{-1}\right)}$$

$$= \left[\left.\frac{cA}{c\tau+1}\right|_{c=0} + \left.\frac{cB}{1+c\tau+1}\right|_{c=1}\right] \Big/ \left(A + B(\tau+1)^{-1}\right)$$

$$\tilde{c} = \frac{B}{A(\tau+1) + B} \qquad (b)$$

now $\int_0^1 P(c)\,dc = 1$ so $A\int_{c=0}^{0+}\delta(0)\,dc + B\int_{c=1^-}^{1^+}\delta(1)\,dc = A + B = 1$

so $A + B = 1 \qquad (c)$

a, b, c = 3 eqns for $\bar{\rho}$, $\tilde{c}$, A, B eliminate A+B + get $\bar{\rho} = \bar{\rho}(\tilde{c})$

$$\boxed{A = \frac{1-\tilde{c}}{(\tilde{c}\tau+1)}} \qquad \boxed{B = \frac{\tilde{c}(\tau+1)}{(\tilde{c}\tau+1)}}$$

solve the $\tilde{c}$ equation for $\tilde{c}$ at every CFD grid point, then use these to get A, B

ex. how compute $\bar{\rho}$ as a function of $\tilde{c}$:

$$\bar{\rho} = \int \rho_R (c\tau+1)^{-1}\left[A\,\delta(c-0) + B\,\delta(c-1)\right]dc$$

so $\bar{\rho} = \left[A\,(c\cdot(0)+1)^{1} + B\,(\tau+1)^{-1}_{c=1}\right]\rho_R$

$= \left[A + B(\tau+1)^{-1}\right]\rho_R$ insert A+B

$$\bar{\rho} = \frac{1-\tilde{c}}{(\tilde{c}\tau+1)} + \frac{\tilde{c}(\tau+1)}{(\tilde{c}\tau+1)}\frac{1}{(\tau+1)}$$

$$\therefore \boxed{\bar{\rho} = (\tilde{c}\tau+1)^{-1}\rho_R}$$

in CFD eqns. replace $\bar{\rho}$ with this - eliminate one unknown
$\tilde{c}$ still an unknown

ex. suppose we want $\bar{c}$ in terms of $\tilde{c}$ (don't need it to close eqns)

$$\bar{c} = \int_0^1 c\, P(c)\, dc = \int c \left[A\,\delta(0) + B\,\delta(1)\right] dc = cA\Big|_{c=0} + cB\Big|_{c=1}$$

$$\therefore \bar{c} = B = \frac{\tilde{c}\,(\tau+1)}{(\tilde{c}\,\tau+1)} \quad \text{from before}$$

ex. suppose we want $\overline{c'^2}$ in terms of $\tilde{c}$

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

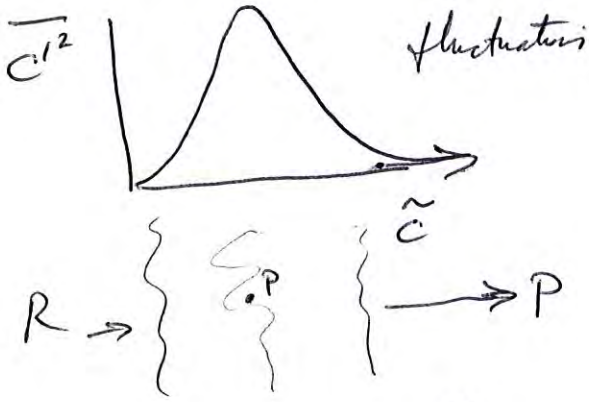
$$= \bar{c}^2 A + (1-\bar{c})^2 B \rightarrow \text{plug in } \bar{c}, A, B \text{ formulas which are in terms of } \tilde{c}$$

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

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

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

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



at point P, thin flamelet is flopping oscillating over point P

where $\tilde{c}=0.5$, about 50% time reactants present, 50% time product

max fluctuations where $\tilde{c}=0.5$

if $\tau=1$ no heat release $c'^2=0$

Summary – Premixed Turbulent Combustion

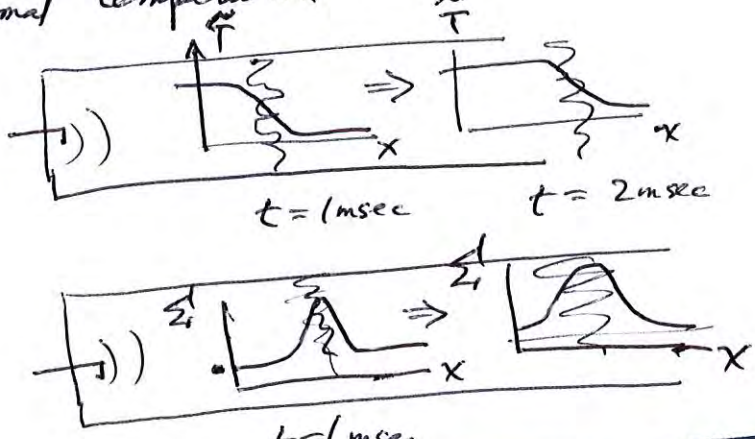
RANS FSD (flame surface density) model

of Bray (Cambridge U.)

$\tilde{c}$ = nondimensional temperature (Favre-averaged)

want to predict

how do $\tilde{T}$ and Σ_1 profiles propagate in space?



solve energy eqn:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{c}\right) + \frac{\partial}{\partial x_k}\left(\bar{\rho}\tilde{u}_k\tilde{c}\right) = \frac{\partial}{\partial x_k}\left(\frac{\mu_T}{\sigma_k}\frac{\partial \tilde{c}}{\partial x_k}\right) + \bar{\dot{\omega}}_R$$

$$\bar{\dot{\omega}}_R = \bar{\rho} I_0 S_{L0} \Sigma_1 \qquad \text{flame surface density } (\Sigma_1) \text{ eqn:}$$

$$\frac{\partial \Sigma_1}{\partial t} + \frac{\partial}{\partial x_k}\left(\tilde{u}_k \Sigma_1\right) = \frac{\partial}{\partial x_k}\left(\frac{\nu_T}{\sigma_{\Sigma_1}}\frac{\partial \Sigma_1}{\partial x_i}\right) + S_1 + S_2 - D$$

$$S_1 = A_{ik}\frac{\partial \tilde{u}_k}{\partial x_i}\Sigma_1 \qquad S_2 = \Gamma_k \frac{\epsilon}{k}\Sigma_1 \qquad D = \frac{\left(S_{L0} + C_1 k^{1/2}\right)\Sigma_1^2}{\text{const}}$$

+ need cons. mass, cons. momentum + k, ϵ eqns

+ need bimodal PDF = $P(c)$

+ need $\bar{\rho} = \int \rho(c) P(c)\, dc$ state relations $\rho(c)$ etc

$\bar{T} = \int T(c) P(c)\, dc$

$\bar{Y}_{H2O} = \int Y_{H2O}(c) P(c)\, dc$ → to get mean species profile

Advantages of CFM (premixed)

1. Includes realistic PDF to account for "turbulence-chemistry" interaction ie. statistics + thermodiffusive effects known to be important (Le) - (propane + methane are different)

2. Includes stretch rate - Flame Stretch
   a) increases wrinkled flame area, ie. Σ'
   b) can use S_L of each flamelet $= S_{L0}(1 - K_a M_a)$ to account for chemistry of HC reaction, extinction
   c) models creation, transport + destruction of surface area
   avoids problem of $\frac{S_T}{S_L} \sim \sqrt{1 + \left(\frac{u'}{S_L}\right)^2}$ which requires S_T due to only local value of u'

ex. $u' = 0$ — also wrinkled in real life — S_T large — algebraic formula invalid but (CFM valid)

u' = large — wrinkled S_T large — algebraic formula valid (CFM valid here too)

3. flamelets — assumes thin — agrees w/ observation

4. K-ε eqns allow turbulence to be created where mean flow gradient are large + be transported elsewhere!

realistic idea - adequate turbulence model

and

CFM is a RANS model } can be easily applied to complex geometries (KIVA)
- burner, counterflow, V-flame with turbulence
- engines, spherical flames
- gas turbines

4. chemistry is OK – zonal approach

– all HC chemistry is inside thin flamelet, contributes to value of S_L

– can say $S_L = S_{L0}(1 - Ka\ Ma)$

– NO_x chemistry – ignore thin flamelet – allocated lean, hot products, post-processing

– (CO ~~soot~~) chemistry – should not be much for lean premixed flames, but it is not in there; predicts zero.

– soot chemistry – can be added on post processing, but not in there yet.

5. predicts realistic S_T turb. burning velocity, if a few constant are "tuned"

6. each term can be measured – important!

Σ, flamelet thickness, k, S_T, $\tilde{u}$, etc.

(only one that can't is ϵ)

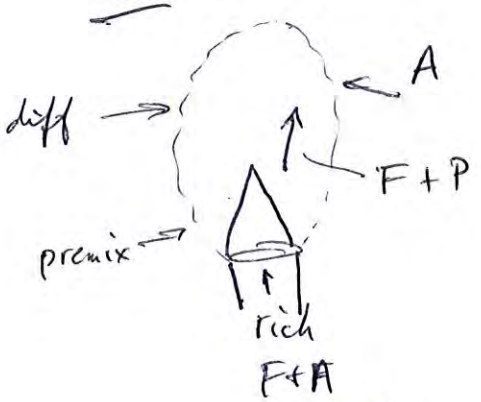
~~7. Can handle premixed + nonpremixed simultaneously~~

7. predicts "bending" of S_T curve due to destruction term (D)

sets up a framework for "partially premixed" = flames that contain premixed and non premixed flames simultaneously which interact = share heat and radicals

solve both $\tilde{c}$ and $\tilde{f}$ eqns (reactedness, mixing)

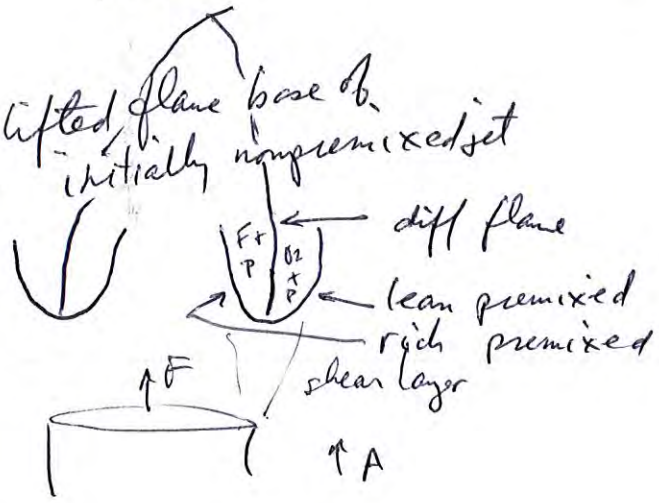
ex. rich bunsen flame



if two flames far apart + don't interact – treat as two separate flames – not "partially premix"

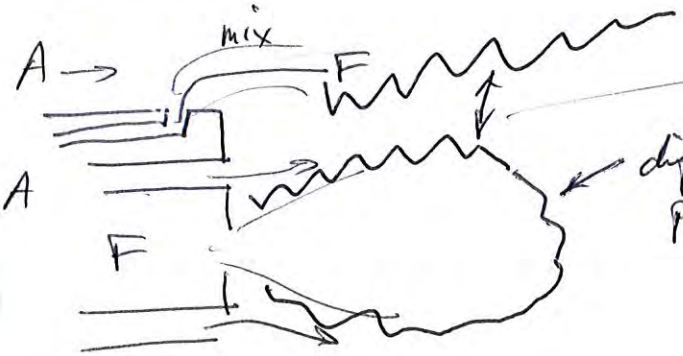
if two flames close, then share heat, radicals + properties of one depend on other = "partially premixed

ex. lifted flame base of initially non premixed set



triple flame = partially premixed

GE gas turbine



premixed (MAIN) – not anchored near wall premix ahead of flame

two flames share heat + radicals

diff. flame – anchored near wall

PILOT

no premixing

partially premixed

Limitations of CFM

1. PDF = 2 fcns – limited to flamelet regime
   need another approach (WSR's ↑ Popt) (predict shape of PDF (lots of uncertainties)
   in ~~high~~ distrib reaction zone
   = difficulty handling large scale unsteadiness
2. RANS – so assumes stationary (steady) turbulence
   if large scales highly unsteady (vortex shedding)
   would be geometry-dependent

   but RANS terms not geometry dependent – steady

   ~~LES~~ better for { combustion instabilities; BB vortex shedding; precessing Recirc Zones gas turbine; highly swirled, IC engines

   RANS best for – single jets, coaxial jets } anything that does not pulse
   flame in bl.

3. Chemistry is limited { major species OK; NOx OK; CO, aromatics, soot – not OK

4. Turb. burn velocity S_T : main test of model
   OK if adjust constants
   want constants that are universal for a given general geometry ie: spherical / IC engines
   conical / gas turbines
   + V-flames
   rear walls – CFlows

5. Cannot yet handle partially premixed
needs work

$I_0 = ?$

4 is $S_L = S_{L0}(1 - Ka\,Ma)$? what Ka, Ma ?

2 source terms S_1, S_2, D correct ?

3 flame extinction ? – locally + globally (at wall)

1 initial conditions for ξ' ?, ϵ ?

(5) model for flame vortex interaction good idea ($T_K \neq ?$ but needs expt. improvement (Adam)

(16) ϵ ~~[illegible]~~ boundary conditions questionable
ξ' "

(17) flame transition from laminar kernel to fully turbulent – ?

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Coherent Flamelet Modeling of Diesel Engine Combustion

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ABSTRACT—A turbulent combustion model based on the coherent flamelet model was developed in this study and applied to diesel engines. The important physics involved in each phase of diesel engine combustion were defined and modeled as directly as possible. The combustion event was broken into three phases: low temperature ignition kinetics, high temperature premixed burn kinetics, and diffusion burn. Two transition steps were developed to model the progression of combustion between each of these phases. The ignition phase was accomplished using the Shell ignition model. The transition to the high temperature premixed burn kinetics was accomplished using a criteria based on heat release rate and temperature. The high temperature premixed burn kinetics were modeled using a global Arrhenius equation for the rate of reaction. The transition to the diffusion burn was based on a critical Damköhler number. Finally, the coherent flamelet model was used as a foundation for the diffusion burn portion of the model. The model was implemented into the multidimensional computational computer code KIVA-II. The sensitivity of the combustion events to several of the model parameters was examined and the results were used to pick the optimum settings for the model. Previous experiments on a Caterpillar model E 300, # 1 Y0540 engine, a Tacom LABECO research engine, and a single cylinder version of a Cummins N14 production engine were used to validate the cylinder averaged predictions of the model. The characteristics of the modeling approach were also addressed by examining the spatial resolution of the model results inside the engine cylinder. The location and magnitude of model heat releases, flame areas, and equivalence ratios were examined. The results of this approach to the modeling of diesel engine combustion could be used to enhance to modeling of engine emissions.

Key Words: Flamelet modeling, diesel combustion

NOMENCLATURE

a	Stoichiometric coefficient of global reaction
A	Pre-exponential constant in Arrhenius equations
A_{Flame}	Flamelet area
C_P	Fluid specific heat
C_1, C_2	Integration constants
D	Laminar mass diffusion coefficient/differential operator
Da	Damköhler number
E_A	Activation energy in Arrhenius equation
h	Heaviside function/rate of heat release per unit flame area
k	Turbulence kinetic energy term of $k-\varepsilon$ turbulence model/thermal conductivity
$\dot{m}''$	Bulk mass flux of fluid per unit flame area at the flame front
MW	Molecular weight
$\dot{q}$	Heat release rate
R	Universal gas constant
R_I	Critical ratio of ignition and premixed heat release rates

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3.4 *Transition to the Diffusion Burn*

The transition to the diffusion burn occurs when the chemical kinetics become very fast compared to the rate of mixing, and the fuel no longer has time to mix with the oxygen before combusting. This transition is accomplished using a critical Damköhler number criteria. The *Da* is defined as:

$$Da \equiv \frac{A \exp(-E_A/RT)}{\varepsilon/k} \tag{6}$$

The constants A and E_A are the same as the constants in the premixed reaction rate. The critical *Da* used in this analysis is 50. Once the critical *Da* is reached locally, a transition to the diffusion burn occurs, and a diffusion flame is initiated. In a diesel engine, the local sources of fuel are the spray droplets, and so at the transition, any droplets which are in a cell which qualifies for transition are flagged to be "diffusion burning" droplets. These droplets then become surrounded by a diffusion flame. As discussed above, this is the mechanism which cuts off the source of fuel for the premixed fuel species. Thus, returning to Equation (4), the source term to due spray evaporation is zero for any droplet or parcel which has undergone the transition to diffusion burn.

It is possible for droplets which have been flagged as diffusion burning to be convected into regions where the *Da* is below 50. These droplets remain diffusion burning droplets due to the high temperature of the diffusion flame which keeps the local sub-grid *Da* near the flame front above the critical transition.

The flame area must also be initialized during the transition. Since this formulation uses droplets as the source of fuel for the diffusion flame, it is reasonable to use the area of the droplets as an initial flame area. The model however does not treat combustion as droplet burning. The area of the droplets is simply used to start the diffusion flame, and the droplets are found on the fuel side of the flame. The model has been found to be relatively insensitive to the initial level of flame area. Once the transition occurs, both the premixed burn and the diffusion burn may occur simultaneously in a cell, with the premixed burn restricted to the oxidizer side of the diffusion flame.

3.5 *The Diffusion Burn*

It is necessary to introduce the coherent flamelet model in its simplest form, i.e. for a classical strained diffusion flame before the complex diesel combustion processes are addressed. A modified version of the coherent flamelet model is used for diesel engine combustion.

3.5.1 *Local Laminar Diffusion Flamelet Analysis*

The coherent flamelet model treats combustion as a group of laminar flamelets which are imbedded in a turbulent flow field. A transport equation yields a global picture of the flame combustion, and the local analysis of the flame sheet yields the rate of reaction per unit flame area. The overall reaction rate is found by integrating the local reaction rate per unit area over all of the flame area and is given by

$$\dot{\rho}_i = \rho_{i,\infty} V_{D,i} \Sigma \tag{7}$$

defines this to be reaction rate

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where $\rho_{i,\infty}$ is the reactant species density far from the flame front, $V_{D,i}$ is the volume rate of consumption of that reactant per unit flame area, and Σ is the local flame area density. As derived in Section A of the Appendix, the local volume rate of consumption per unit flame area is:

$$V_{D,f} = \frac{\bar{\rho}\bar{D}\dfrac{dY_f}{dx}}{\rho_{f,\infty}} = Y_{f,+\infty}\frac{\bar{\rho}}{\rho_{f,\infty}}\sqrt{\frac{\varepsilon_s\bar{D}}{2\pi}}\frac{(\Phi+1)}{\Phi}\exp\left[-\left(\mathrm{erf}^{-1}\left(\frac{\Phi-1}{\Phi+1}\right)\right)^2\right] \tag{8}$$

Here, $Y_{f,+\infty}$ is the mass fraction of the fuel far away from the flame and the equivalence ratio Φ is the ratio of the total amount of fuel present to the amount of fuel required to completely combust all of the oxygen present. The equivalence ratio for the diffusion flame is based on the reactant concentrations far from the flame front. The volume rate of consumption of the oxidizer can also be found, using the fact that the reactants diffuse in stoichiometric proportions into the flame front. Since $V_{D,f}$ has units of velocity, it is often referred to as a diffusion velocity (Marble and Broadwell, 1977). The energy equation can also be solved to yield an estimate of the flame temperature (Musculus, 1994). This is especially useful for emissions predictions which rely heavily on temperature distributions.

3.5.2 *Flame Area Transport Equation*

The global flame area density in the coherent flamelet model is defined as

$$\Sigma = \frac{\delta A}{\delta V} \tag{10}$$

where Σ, the flame area density, is a scalar which is imbedded in the flow field. For convenience, a new variable is defined for transport such that

$$S = \bar{\rho}\Sigma \tag{11}$$

With some manipulation using this substitution, the transport equation for flame area then becomes:

$$\frac{\partial}{\partial t}\tilde{S} + \nabla\cdot(\tilde{S}\tilde{u}) = \nabla\cdot\frac{\mu_{\text{turb}}}{\sigma_s}\nabla\frac{\tilde{S}}{\rho} + \bar{\rho}\left.\frac{d\tilde{\Sigma}}{dt}\right|_{\text{Production}} - \bar{\rho}\left.\frac{d\tilde{\Sigma}}{dt}\right|_{\text{Destruction}} \tag{12}$$

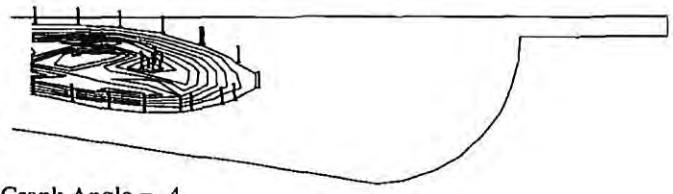
flame surface density balance

Now, the derivative term $d\tilde{\Sigma}/dt$ must be evaluated. It has been proposed that the behavior of an incremental unit of flame area which is subjected to some strain due to the flow mechanics and can be represented by (Candel *et al.*, 1990; Musculus, 1994):

$$\left.\frac{d\tilde{\Sigma}}{dt}\right|_{\text{Production}} = \alpha\tilde{\varepsilon}_s\tilde{\Sigma} \tag{13}$$

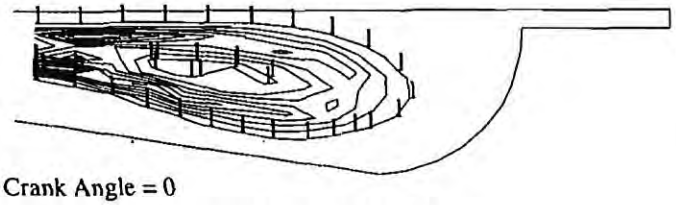
where α is a model constant and $\tilde{\varepsilon}_s$ is the strain rate induced on the flame surface by the fluid.

The strain rate term $\tilde{\varepsilon}_s$ can be found by a several methods. The turbulent strain rate is usually dominant, and is most often the factor used in determining the strain rate (Candel *et al.*, 1987; Marble and Broadwell, 1977; Cheng *et al.*, 1991; Duclos *et al.*,



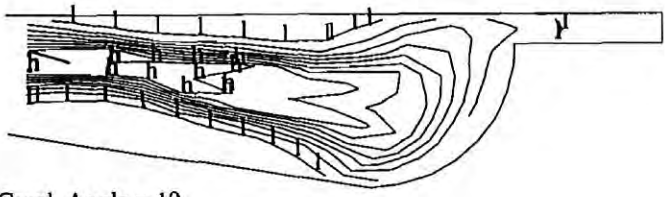
Crank Angle = -4

Low = 34.98, High = 314.81 (cm^2/cm^3)



Crank Angle = 0

Low = 46.86, High = 421.75 (cm^2/cm^3)



Crank Angle = 10

Low = 22.57, High = 197.60 (cm^2/cm^3)

FIGURE 8 Flame area density (Sigma), across center of spray.

4. variation of the form of the production term
5. addition of a critical premixed equivalence ratio
6. examination of the necessity of the premixed fuel transport equation
7. examination of the necessity of the inerts transport equation
8. elimination of reactant combustion near the diffusion flame

A Tacom LABECO research engine (Table I) was used as a basis for this entire sensitivity study. A summary of the effects of each of the above tests can be found in Table II (also see Musculus, 1994). The cylinder pressure was measured in the experiment, and a heat release curve was derived from the experimental pressure trace though the use of a zero-dimensional simulation code (Van Gerpen, 1984). The cylinder pressure predicted by the model was mass averaged over the entire domain, and the

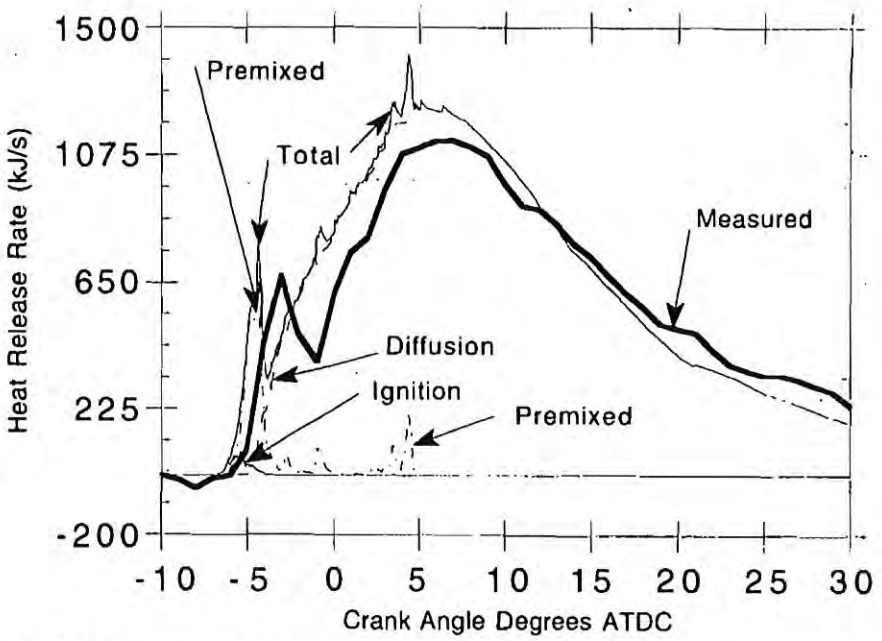


FIGURE 17b The ignition, high temperature kinetics (premixed), and diffusion burn components of the computational heat release and the measured (from experimental pressure trace) heat release for the Tacom engine.

temperature kinetics. Also, the ignition model is only used at temperatures below 1050 K. As the combustion proceeds, the cylinder temperature quickly becomes higher than this cutoff level in almost the entire volume, and thus the ignition model is not active.

The shape of the premixed burn curve mimics the experimental heat release spike quite well. It is this spike which is responsible for the kink in the pressure trace. Note that the area under the curve for the computational heat release during this spike is not as large as that of the experimental heat release. This is the reason that the computational kink in the pressure curve is not as large as that of the experiments.

The qualitative shape of the diffusion burn heat release is predicted quite well. However, the modeled diffusion burn heat release occurs sooner than the experimental curve. This is due to the inadequate computational premixed burn. When the kink in the pressure trace is not matched well, the diffusion burn must be modified if the correct peak pressure is to be reached. Since the constants of the diffusion burn model are found by matching these experimental pressure curves, they were adjusted in such a way as to compensate for the inadequate premixed burn. Thus, the early heat release for the diffusion burn must be quite large to compensate for a low premixed burn. Later, the fuel becomes exhausted and the computational heat release becomes smaller than the experimental heat release.

Modeling of Combustion in Gasoline Direct Injection Engines for the Optimization of Engine Management System Through Reduction of Three-Dimensional Models to (n×One-Dimensional) Models

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Gasoline direct injection (GDI) spark ignition engines may be able to run over a wide range of operating conditions. The GDI process allows combustion with lean mixtures which may lead to improved fuel economy and emissions relative to homogeneous spark ignition (SI) engines. To satisfy the different modes of operation, the tuning of GDI engines requires a large number of engine tests which are time-consuming and very expensive. To reduce the number of tests, a model with a very short computational time to simulate the engines in the whole operating range is needed; therefore the objective of this paper is to present a reduced model to analyze the combustion process in GDI engines, applied to a homogeneous stoichiometric mode. The objective of the model is to reproduce the same tendencies as those obtained by three-dimensional models, but with a reduced computational time. The one-dimensional model is obtained thanks to a reduction methodology based on the geometry of the combustion front computed with three-dimensional models of the KIVA-GSM code, a modified version of KIVA-II code including a CFM combustion model. The model is a set of n one-dimensional equations (i.e., for n rays), taking into account a thin flame front, described with the flamelet assumption. It includes a CFM combustion model and a (k,ε)-model including the mean air motions (swirl and tumble). The results of the one-dimensional model are compared to those obtained by the KIVA IIGSM under different engine conditions. The comparison shows that the one-dimensional model overestimates the maximum cylinder pressure, which has an insignificant effect on the net indicated work per cycle. The results obtained by the numerical simulations are close to those given by the three-dimensional model, with a much reduced computation time. [DOI: 10.1115/1.1570859]

Coherent Flamelet Model

1 Introduction

The gasoline direct injection (GDI) engine offers a multitude of potential advantages which may lead to improved emissions and fuel economy relative to port injected spark ignition (SI) engines. Especially at part load conditions, the GDI engines are able to run in a stratified charge mode which combines the benefits of lean combustion with a nearly throttle free operation. This is the major step in overcoming the principal disadvantages of SI engines compared to diesel engines. Furthermore, the GDI process has no delay in fuel transport during cold start, warm up, and transient mode, which leads to combustion with lean mixtures and reduced HC and CO emissions. At full load operation, the combustion system is switched to the homogeneous stoichiometric mode, and to purge the NO_x catalyst the combustion system is switched to a rich mode (equivalence ratio greater than one, generally fixed around 1.3). The gasoline direct injection engines are thus able to run over a wide range of operating conditions (homogeneous stoichiometric, homogeneous lean, stratified lean).

Generally, three-dimensional models are used to understand different phenomena and to analyze the in-cylinder processes for the optimization of the combustion chamber design. These three-dimensional models implemented in different codes (KIVA or Star-CD for example) require many hours on a high end computer, to compute a combustion phase for one cycle and are not suited to assist the engine tuning. Today, the car manufacturers need models with a very short computational time to simulate the engine in the whole operating range; this step is very important for the engine tuning, to reduce the number of engine experiments on the engine test bench, which are very expensive.

The objective of this study is to provide the car manufacturers with a simple physical combustion model to assist engine tuning and engine management system optimization, with the aim of air-fuel ratio and performance control over the whole engine operating range. It has to be calibrated on a few operating points, using

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Table 1 Engine geometry

Bore	82.7 mm
Stroke	93 mm
Connecting rod length	144 mm
Displaced volume	1998 cm^3
Compression ratio	10

$$\frac{\partial \Sigma}{\partial t} + \mathrm{div}(\vec{u}\Sigma) = \mathrm{div}\left[\left(\lambda_\Sigma \bar{\rho}\bar{\kappa}\frac{\bar{\kappa}}{\bar{\varepsilon}} + \frac{\mu_t}{S_c}\right)\overrightarrow{\mathrm{grad}}\left(\frac{\Sigma}{\bar{\rho}}\right)\right] + \alpha_\Sigma(\bar{\kappa}_t + \bar{\kappa}_L)\Sigma - \beta S_L\frac{\Sigma^2}{(1-\bar{c})} + \phi_\Sigma$$

has a nonlinear term on the right-hand side written as follows:

$$f(\Sigma) = \Sigma\left(\alpha_\Sigma(\bar{\kappa}_t + \bar{\kappa}_L) - \beta S_L\frac{\Sigma}{(1-\bar{c})}\right)$$

which has the same structure as the general form of Eq. (4) (Fisher-KPP equations, [15]). Then the equation for Σ takes into account the propagating front in the combustion chamber and more precisely a thin flame front which delimits the fresh gas zone and the burned gas zone.

The equation of the dissipation rate of the turbulent kinetic energy written as follows (from KIVA-GSM):

$$\frac{\partial \bar{\rho}\bar{\varepsilon}}{\partial t} = \mathrm{div}(\bar{\rho}\vec{\tilde{u}}\tilde{\varepsilon}) = \mathrm{div}\left[\left(\lambda_\varepsilon \bar{\rho}\bar{\kappa}\frac{\bar{\kappa}}{\bar{\varepsilon}} + \frac{\mu_t}{S_c}\right)\overrightarrow{\mathrm{grad}}\,(\tilde{\varepsilon})\right] + (C_1 G_k - C_2\bar{\rho}\bar{\varepsilon})\frac{\bar{\varepsilon}}{\bar{\kappa}} - C_3\bar{\rho}\bar{\varepsilon}\,\mathrm{div}(\vec{\tilde{u}})$$

has also on the right-hand side a nonlinear term which can be written as

$$f(\bar{\varepsilon}) = (C_1 G_k - C_2\bar{\rho}\bar{\varepsilon})\frac{\bar{\varepsilon}}{\bar{\kappa}},$$

the latter also has a structure similar to the Eq. (4). We can note here that there is a second front in the combustion chamber. Consequently, we observe two fronts: the first one which we called the «chemical front» or «combustion front» due to the equation for Σ and the second one the «turbulent front» due to the equation for ε. We can find here an analogy with the zero-dimensional models of Keck [16] and Tabaczynski [17], which take into account a chemical front in the form of a volume of burned gas, and a turbulent front in the form of gas carried by the flame.

2.4 Numerical Observations. We have used the results obtained from the KIVA-GSM code applied to the Renault F5R direct injection gasoline engine to observe the trace of the two fronts extracted with the level set method. The engine geometry is described in Table 1 and the combustion chamber is shown on Figure 1.

Two operating conditions have been chosen, in order to be representative of the engine conditions in the vehicle:

- part load at 2000 rpm, equivalence ratio 1, ignition timing 18 deg CA (BTDC).
- full load at 5000 rpm, equivalence ratio 1.11, ignition timing 18 deg CA (BTDC).

The observation of the different fronts has been set up from the different plots along one ray, from the spark plug to the piston.

Chemical Front. The Fig. 2 shows the evolution of the flame surface density obtained at 2000 rpm along one ray. Here from the spark plug to the piston center we observe then the trace of the front. On this figure, at the abscissa 0 (spark plug), we see that there is no longer a flame (only burned gas in this region) and

Fig. 1 Geometry of the combustion chamber

when we follow the ray the front is reached close to the piston shown by the increase of the flame surface density.

We observe the same kind of evolution at 5000 rpm full load. Figures 3–4 show the evolution of the flame surface density for this point and at different times (TDC, 3 deg ATDC); we see on these figures a progress of the flame front with time from the spark plug to the piston along the ray.

Turbulent Front. In order to verify that the behavior is similar for the turbulent kinetic energy dissipation rate, we have plotted on Figs. 5–6 on the same graph at 5000 rpm (TDC, 3 deg ATDC), the chemical front and the turbulent front. A propagating front with time can also be observed for the dissipation rate. The turbulent front is ahead of the chemical front, but both fronts progress at the same speed. This conclusion is independent from the ray orientation; Figs. 7–8 show the progress of both fronts along a different ray, from the spark plug to the cylinder periphery. There also both fronts progress with the same speed, with the

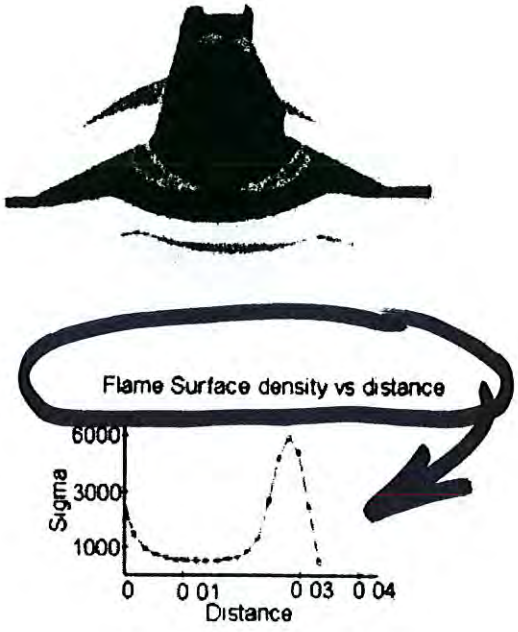

Fig. 2 Reaction rate and flame surface density at part load and 2000 rpm—0 deg crank angle (TDC)

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Development of a Coherent Flamelet Model for a Spark-Ignited Turbulent Premixed Flame in a Closed Vessel

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Three-dimensional calculations of turbulent combustion which include ignition, laminar and turbulent flame propagation and quenching at the wall are performed by the coherent flamelet model (CFM). The existing CFMs in the literature are tested and new forms are proposed. A mean stretch factor I_0 is introduced to consider the stretch and curvature effects of turbulence. Quenching at the wall is simulated by the simple wall flux model (SWFM) of the flame surface density. Two forms of the flame production term, CFM-1 and CFM-2, are tested to show the predictive capability of the CFM for turbulent burning velocity. CFM-1 has the flame production term given by the average rate of strain proposed by Cant et al. [20], while CFM-2 has the production term proportional to the rms turbulent velocity. It turns out that the turbulent burning velocity of CFM-2 is in reasonable agreement with the data of Checkel and Thomas and Bradley's correlation with variation of the Karlovitz number, rms turbulent velocity, and integral length scale. © 1998 by The Combustion Institute

INTRODUCTION

Faster combustion in a reciprocating internal combustion engine has merits in fuel economy and exhaust emissions. Since the turbulent burning velocity increases with increasing turbulence intensity, one of the current design targets is to develop an engine with higher turbulence intensity. The intake port, cylinder head, and piston have complicated three-dimensional geometry to enhance turbulence. Two powerful tools available for engine designers are laser diagnostics for experimental measurement and three-dimensional computational fluid dynamic simulation. Although three-dimensional simulations have become a common practice in the automotive industry, most of these are confined to cold flow simulation. There is, as yet, no satisfactory model for turbulent combustion phenomena in an engine.

A turbulent combustion regime may be specified by the chemical time scale, integral length scale, and turbulence intensity. The chemical time scale is much smaller than the turbulent time scale in many combustion devices so that the laminar flamelet concept is valid [1]. The turbulent combustion models applicable in three-dimensional analysis are the eddy breakup (EBU) model [2, 3], the assumed probability density function (PDF) model [4–6], and the coherent flamelet model (CFM) [7–9]. The EBU model assumes that the mean reaction rate is controlled by the turbulent mixing time with no consideration for chemical effects. The assumed PDF model is applied to turbulent combustion to solve transport equations for the mean and fluctuation of the mixture fraction or reaction progress variable. The CFM views the turbulent flame as a collection of flamelet elements embedded in turbulent flow. The CFM is applicable to both premixed and nonpremixed flame on the basis of the laminar flamelet concept. Its important advantage lies in the decoupled treatment of the chemical reaction and turbulent flow. The concept of CFM originates from Marble and Broadwell [7] who analyzed nonpremixed turbulent flames by the CFM. Cheng et al. [10] simulated combustion in a spark ignition engine by the CFM and examined the sensitivity to major engine parameters. Boudier et al. [11] simulated spark ignition engine combustion using the Intermittent Turbulence Net Flame Stretch (ITNFS) model [12], which took into account the influence of different length scales on flame straining and quenching. Calculated pressure traces were compared with experimental data to assess the CFM. Poinsot et al. [13] suggested a wall quenching model called the Flame Interacting with Surface and Turbulence (FIST) model which assumes

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flame–wall interaction at scales smaller than a computational mesh. Duclos et al. [14] compared turbulent burning velocities of various CFMs with experimental burning velocities and KPP (Kolmogorov, Petrovski, Piskunov) analysis [15] in one dimension. It was shown to be possible to predict deviation from linear increase of the turbulent burning velocity with the rms turbulent velocity due to flame stretch effects.

In this paper the CFM is applied to the ignition and flame propagation phase in an enclosed cubic chamber. Two forms of the flame production term, CFM-1 and CFM-2, are proposed to match the experimental data of Checkel and Thomas [16] and Bradley and co-workers' correlation [17, 18].

LITERATURE REVIEW

The turbulent premixed flame has been viewed as a collection of one-dimensional, planar laminar flamelets since the days of Damköhler (1940). The laminar flamelet regime exists for $Da > 1$ and $K < 1$, where Da is the Damköhler number and K is the Karlovitz number. The Damköhler number Da is defined as the ratio of the integral time scale to the flame time scale as

$$Da = \tau_t/\tau_F \tag{1}$$

$$\tau_t = l_t/u' \tag{2}$$

$$\tau_F = \delta_L/U_L. \tag{3}$$

l_t is the integral length scale. u' is the rms turbulent velocity. δ_L is the laminar flame thickness. U_L is the unstrained laminar burning velocity. The Karlovitz number K is defined as

$$K = \tau_F\left(\frac{1}{A}\frac{dA}{dt}\right), \tag{4}$$

where A is the flamelet surface area. The expression in parentheses in Eq. (4) represents the flamelet stretch rate. The Karlovitz number is computed as

$$K = \frac{u'}{\lambda}\left(\frac{\delta_L}{U_L}\right) = 0.145\left(\frac{u'}{U_L}\right)^2 R_L^{-0.5} \tag{5}$$

$$R_L = \frac{u' l_t}{\nu} \tag{6}$$

TABLE 1

Production and Annihilation Terms in Eq. (8)[a]

	S	D
Cheng [10]	$\alpha\sigma\frac{\epsilon}{k}\Sigma$	$\beta\frac{U_L}{\left(\frac{\bar{Y}}{Y_0}\right)}\Sigma^2$
ITNFS [11]	$\alpha\Gamma_k\frac{\epsilon}{k}\Sigma$	$\beta\frac{U_L + Ck^{1/2}}{\left(\frac{\bar{Y}}{Y_0}\right)\left(1-\frac{\bar{Y}}{Y_0}\right)}\Sigma_2$
CFM-1	$\alpha\sqrt{\frac{\epsilon}{15\nu}}\Sigma$	$\beta\frac{U_L}{\left(\frac{\bar{Y}}{Y_0}\right)\left(1-\frac{\bar{Y}}{Y_0}\right)}\Sigma^2$
CFM-2	$\alpha\frac{u'}{l_{ic}}$	$\beta\frac{U_L}{\left(\frac{\bar{Y}}{Y_0}\right)\left(1-\frac{\bar{Y}}{Y_0}\right)}\Sigma^2$

[a] $\bar{Y}$ = mean fuel mass fraction, Y_0 = fuel mass fraction in the fresh mixtures ($\bar{Y}/Y_0 = Y_1$), $\sigma = 0.5$ in Cheng and Diringer [10].

according to Abdel-Gayed et al. [19]. Here, λ is the Taylor microscale, R_L is the turbulent Reynolds number, and ν is the kinematic viscosity.

The mass burning rate per unit volume in the unstretched laminar flamelet regime is simply given as

$$\dot{w} = \rho_u U_L \Sigma \tag{7}$$

where ρ_u is the fresh gas density and Σ is the flame surface density, the flame area per unit volume. Chemical and molecular effects are represented by U_L, while turbulence effects are represented by Σ.

A conservation equation for the flame surface density Σ is

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial}{\partial x_i}(U_i \Sigma) = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_\Sigma}\frac{\partial \Sigma}{\partial x_i}\right) + S - D, \tag{8}$$

where S is the production of flame surface by turbulent rate of strain, D is the annihilation of flame surface by mutual collision, ν_t is the turbulent kinematic viscosity, and σ_Σ the turbulent Schmidt number ($\sigma_\Sigma = 1$). A main focus of modeling is the production and annihilation terms, S and D, typical forms of which are listed in Table 1. The S term is proportional to Σ in all models in Table 1. It is given as a product of the average rate of strain and the flame surface

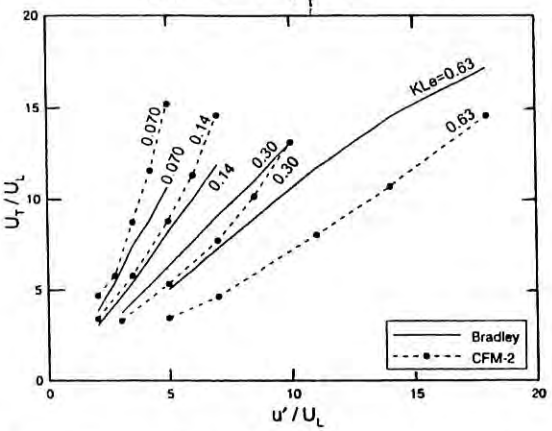


Fig. 10. Turbulent burning velocity vs u'/U_L for correlation of Bradley et al. and CFM-2.

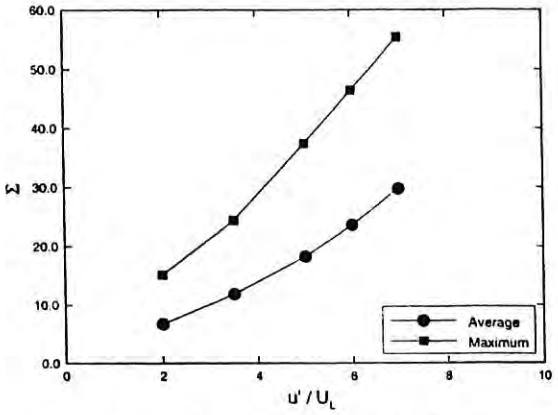


Fig. 11. Average and maximum flame surface density vs rms turbulent velocity of CFM-2 for $KLe = 0.14$.

the incompletely burned region tends to have a bigger effect at higher u', due to the larger value of Σ there. Note that the burned mass fraction in the central region is greater than about 0.9, but never equal to unity in Fig. 7. The total flame surface area, which is the product of the average value of Σ and the chamber volume, determines the global mass burning rate and the pressure rise rate. In Fig. 11 it is shown that the average value of Σ varies with u'/U_L in the same way as the calculated turbulent burning velocity of Fig. 10, while the maximum value of Σ shows an almost linear increase with u'. The turbulent burning velocity is proportional to the maximum value of Σ if the flame front is located at the maximum value of Σ. Better agreement would have been obtained if the turbulent burning velocity had been defined in terms of the flame front instead of the chamber pressure.

Comparison of KPP and Equilibrium Analysis for the Turbulent Burning Velocity

As helpfully suggested by one of the reviewers, the KPP analysis [15] presents a simple analytical procedure to predict the turbulent burning velocity of a given CFM formulation. However, its predictions, listed in Table 4 [14], are not consistent with some of the calculated results in Figs. 3–5 and Figs. 9–10. For example KPP analysis predicts the turbulent burning velocity to be proportional to u' at constant Karlovitz number for Cheng's model and EBU. However, computed results show it to decrease with u' at a constant K, in Fig. 3. It may be due to some of the strong assumptions such as a steady one-dimensional flame involved in KPP analysis in this case.

Another simple analytical procedure is the equilibrium analysis which assumes that the source term balances the sink term in the flame surface density transport equation during steady flame propagation. In spherical flame propagation the ratio of the source and sink term may be greater than unity because there must be continuous net generation of flame surface. The equilibrium assumption has been tested for different values of u' in Fig. 12 for the case of KLe fixed equal to 0.14, as in Fig. 3, by CFM-2. The ratio of the integrated source and sink term

TABLE 4

Variation of Turbulent Burning Velocity with Respect to Turbulence Condition as Predicted by KPP Analysis

Case	EBU	Cheng	ITNFS	CFM-1	CFM-2
Constant K	u'	u'	$\sqrt{\Gamma_k}u'$	$u'^2/\sqrt{K}$	$u'^{2.5}/K$
Constant l_t	u'	u'	$\sqrt{\Gamma_k}u'$	$u'^{1.25}$	u'
Constant u'	constant	constant	$\sqrt{\Gamma_k}$	$l_t^{0.25}$	$\sqrt{l_t}$

go over Muscular + Rutland

- includes spray
* - identifies spatial location of { lam kernel burn vs t; premix burn vs (t); diffusion " (t)
" " "

* - shows heat release rate ~> p (t) has two spikes, in agreement with expt

* - gives profile of $\tilde{\xi}$ vs (x, y, z, t)

- have complex geometry

- realistic chemistry → $S_L(\phi, P, T)$

- all of * can be compared to expt!

* - ~~varies~~ he does sensitivity study = Varies 3 constants in CFM model
  - large scale stretch term constant
  - destruction term constant
  - critical Da for transition premix → diff burn
  - etc

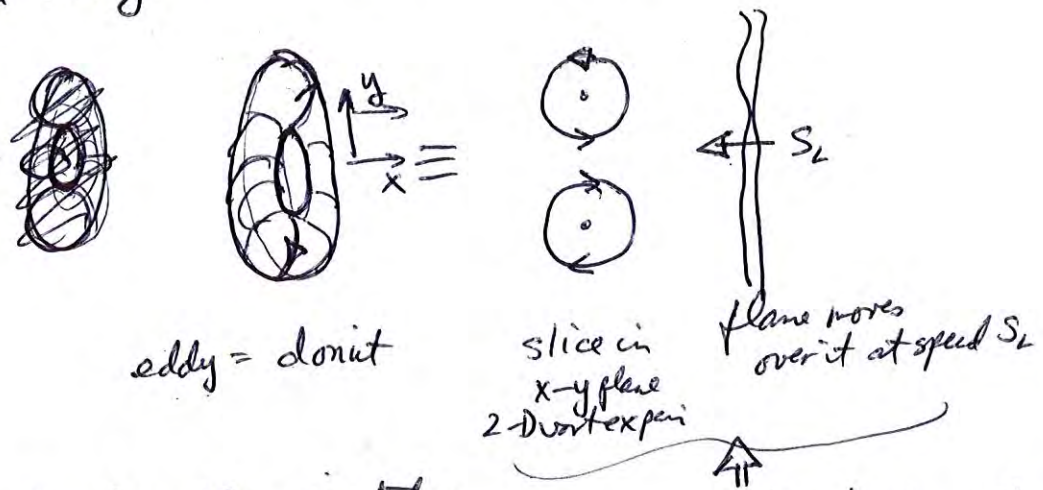
good thing = many intermediate things can be compared to expt, including δ_T burnt thickness

however = he only compared p(t) to expt here

Stretch efficiency function

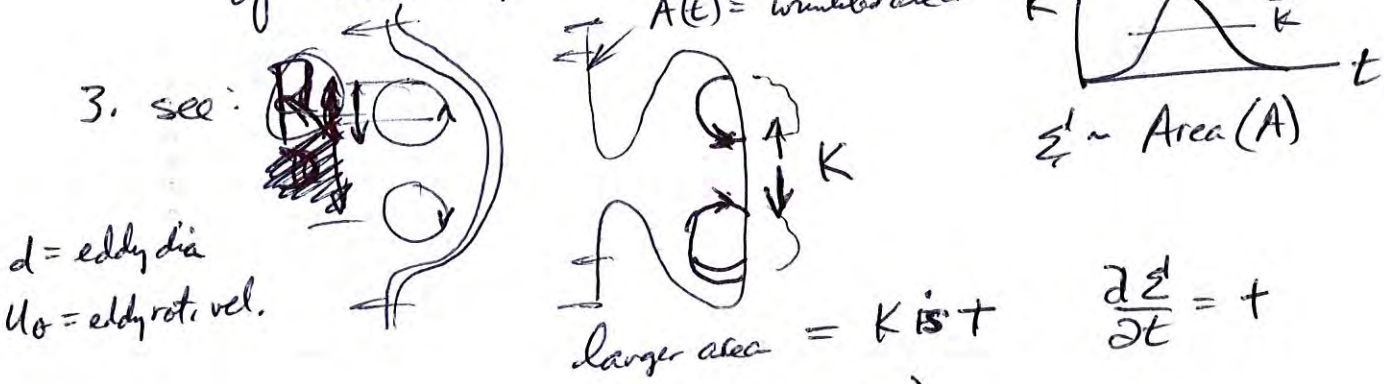
$\Gamma_K = ?$ Meneveau and Poinsot CNF 86, 311, 1991

1. assume "eddies" is toroidal vortex ⇒ flame moves over it at S_L



2. run laminar flow simulation of laminar flat flame moving over 2-D laminar vortex pair

3. see:



4. verify using expts (Mueller + Driscoll)

5. for this eddy we get $\frac{\partial \Sigma'}{\partial t} = \left(\Gamma_K \frac{u_\theta}{R}\right)\Sigma'$

$\frac{\partial \Sigma'}{\partial t}$ (measured)

contrib to Γ_K

$\frac{u_\theta}{R}$: rot. velocity of eddy (measured); R ~ vortex radius (see above)

$$\bar{K} \sim (d\Gamma_K)\frac{u_\theta}{R}$$

get $(d\Gamma_K)$ for this eddy size (R) for this eddy strength (u_θ)

avg in time (measure it) (compute it)

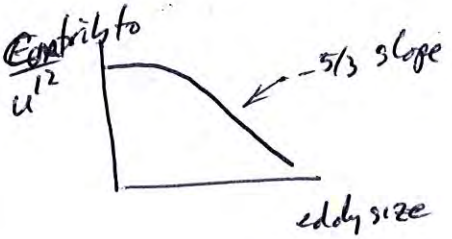
assume or known in computation ⇒

$$K = -\bar{n}\cdot(\bar{n}\cdot\bar{\nabla})\bar{u} + \bar{\nabla}\cdot\bar{u} + S_L/R_c$$

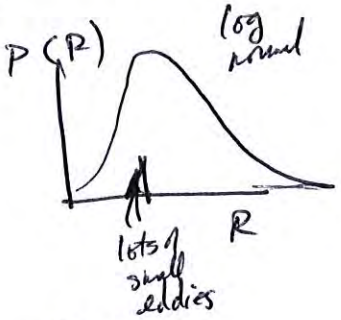
7-41

6. repeat computation (or expt) for
   - many eddy sizes (ℓ), strengths (u_ℓ)

7. assume Kolmogorov distribution of eddy sizes, strengths



$$\frac{(u')^3}{\ell} = \frac{u_\ell^3}{d}$$

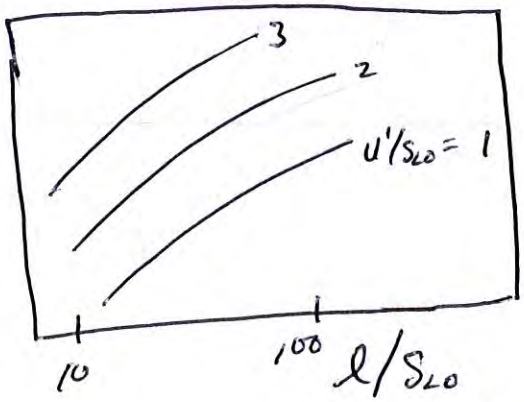


8. $\Gamma_K = \int d\Gamma_K \qquad d\Gamma_K = f(u_\ell, d)\, du_\ell\, dR$

sum over all eddy sizes, strengths

$$\therefore \Gamma_K = f\left(\left(u'/s_{L0}\right), \ell/\delta_{L0}\right)$$

u'/s_{L0}: rms vel. fluct / lam burn vel ; ℓ/δ_{L0}: integral scale / lam flame thickness



computed values of stretch eff. function

∴ larger, stronger vortices are more efficient at wrinkling flame smaller, weaker vortices!

9. repeat all this for real eddies measured in a turbulent flame — Adam Steinberg

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.

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How well can we model premixed turbulent flames ?

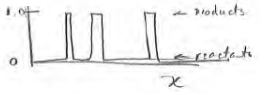
Bray / FSD model

Assume thin or thickened wrinkled flamelets

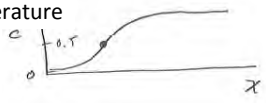
fully premixed or stratified premixed, FSD model is being modified to handle partially-premixed

considers corregated (pockets) flamelet merging stretch rate increases area

Gas temperature



Mean temperature



Σ = FSD

Masuya, Bray, Comb Sci Tech 25, 127

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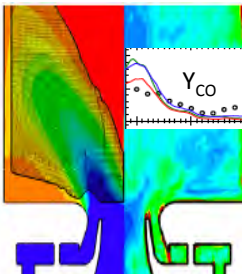
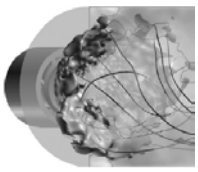
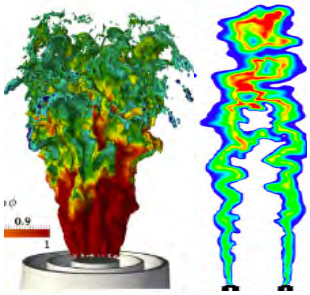
Who is using the Bray / FSD LES method ?



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 $\rho = p/RT$, it follows that inserting the above in for T yields:

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

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

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

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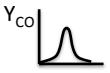
Bray / FSD LES model – of premixed turb. flames

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

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

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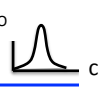
State relations - between instantaneous Y_{CO}, ρ, etc. and c from lam. flamelet equation

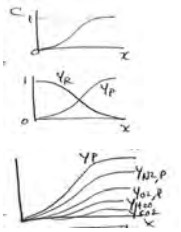


c = reactedness
Y_P = mass fraction products

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

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

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



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

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

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

show that $Y_{CH4} = 0.062\,Y_R = 0.062\,(1\text{-}c)$ 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.

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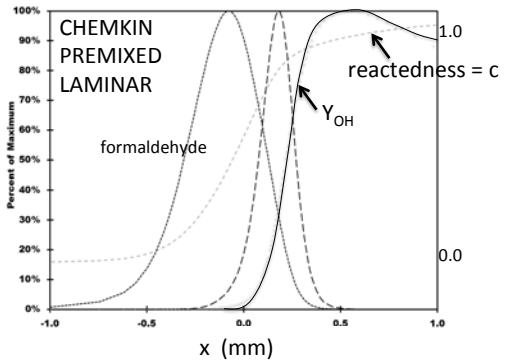
State relations: between Y_i , ρ, T and reactedness c



PREMIXED state relation from CHEMKIN premixed unstrained flamelet

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

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Conservation of mean reactedness

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

(kg/m³) (m/s) (1/m) = (kg/m²/s) (area/vol)

reaction rate/area

rate of temperature rise in x direction

turbulent flux of temperature fluctuations

volumetric reaction rate kg/s of products /m³

Conservation of scalar flux

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

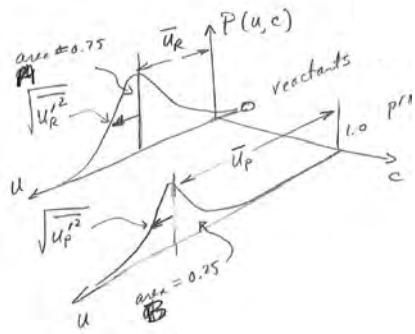
$$= -\overline{c''}\frac{d\bar{p}}{dx} + \overline{u''w} - \bar{\chi}_{uc}$$

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)

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



δ(c) is delta fcn centered at c = 0
δ(1-c) is delta fcn centered at c = 1

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

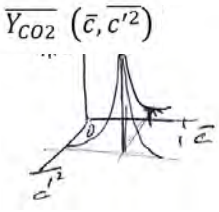
Areas under Gaussians A + B = 1

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

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



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 δ(c-0) + B δ(c-1)

example

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

$$= \bar{c}^2 A + (1-\bar{c})^2 B \rightarrow \text{plug } \bar{c}, A, B \text{ formulas with each in terms of } \tilde{c}$$

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

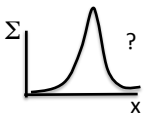
$$\overline{c'^2} = \frac{\tilde{c}(1-\tilde{c})(\tau+1)}{(\tilde{c}\tau+1)^2}$$

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

$\tilde{c}=1$ pure products, $\overline{c'^2}=0$

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

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

Flame Surface Density Conservation Equation

mean stretch rate $K = (u' / L)\;\Gamma$ causes flame area to increase
flamelet merging term $A\,\Sigma^2$ causes flame area to decrease

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

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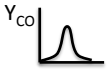
Bray / FSD LES model – of premixed turb. flames

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

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

"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

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Bray / FSD model applied to premixed jet flame

Prasad and Gore
Comb Flame 116,1

Mean Reactedness $\tilde{c}$

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

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 $\tilde{u}$

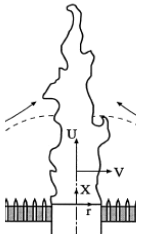
$$\frac{\partial \bar{\rho}\tilde{u}^2 r}{\partial x} + \frac{\partial \bar{\rho}\tilde{u}\tilde{v} r}{\partial r} = rg(\rho_\infty - \bar{\rho}) + \frac{\partial}{\partial r}\left(r\mu_t\frac{\partial \tilde{u}}{\partial r}\right)$$

Continuity For $\tilde{v}$

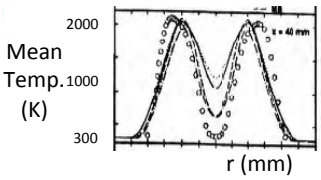
$$\frac{\partial \bar{\rho}\tilde{u} r}{\partial x} + \frac{\partial \bar{\rho}\tilde{v} r}{\partial r} = 0$$

TKE for k, ε

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



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



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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

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

58

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 $\mathbf{S_{T,\Delta}}$

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

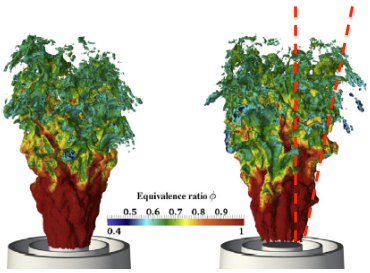
Ξ = new flame surface density parameter

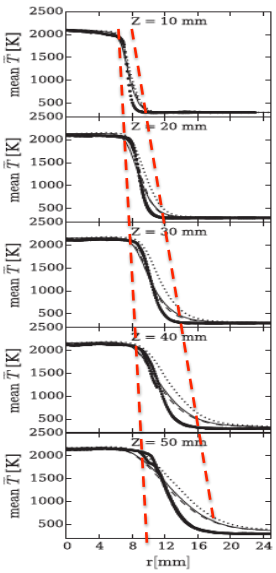
Solves for mean progress variable $\widetilde{Y_c}$

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

59

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

60

Motivation– kilohertz imaging

Cam Carter (AFRL)
Tonghun Lee (UIUC)
10 kilohertz CH
Reaction layer
Applied Optics B 116: 515

Steinberg, Driscoll
Michigan kHz PIV
eddies passing
through flame
Comb Flame 156, 2285

9

Best current models ?

PREMIXED LES			React Rate	authors
1	**FSD**	Flame surface density, also called F-TACLES = tabulated chemistry LES	FSD eqn w flamelet state relns	Bray, Vervisch Veynante, Fureby Ihme,
2	**FPV**	Flamelet progress variable	flamelet state relns	Moin, Ihme Pitsch, Kempf
3	**TFM**	Thickened flamelet model	flamelet	Poinsot
4	**CMC**	Conditional Moment Closure	flamelet	Swami, Huh
5	**G Eqn**	G equation	G-Eqn	Pitsch, Bai
6	**LEM**	Linear eddy model	LEM	Menon
NON PREMIXED LES				
1	**SSLF**	Steady strained laminar flamelet Z eqn with scalar dissipation rate	strained flamelet	Peters, Pitsch
2	**FPV**	Flamelet progress variable Z and c eqns	flamelet state relns	Moin
3	**CMC**	Conditional Moment Closure	flamelet	Bilger, Masri
4	**PDF**	PDF transport method	parcels	Pope

10

References – Premixed models

- **FSD = Flame surface density LES models F-TACLES**
  Mercier, Veynante, PROCI 35, 1259, Hawkes, Cant, Comb Flame 126, 1617
  See, Ihme, PROCI 35, 125, Duwig, Flow,Turb Comb 79, 433

FPV = Flamelet progress variable
Pierce, Moin, J. Fluid Mech 504-73, Chen, Ihme Comb Flame 160, 2896
Lamouroux, Ihme, Comb Flame 161, 2120

TFM = Thickened flamelet model
Selle, Poinsot, Comb Flame 137, 489, Esclapez, Cuenot, PROCI 35, 3133
De, Acharya, Comb Sci Technol 181, 1231

CMC = Conditional Moment Closure
Amzin, Swaminathan, Comb Sci Tech 184, 1743, Amzin Cant, Comb Sci Tech 187, 1705

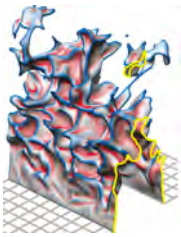
G-Equation
Knudsen, Pitsch, Comb Flame 159, 242, Nogenmyr, Comb Flame 156, 25

LEM = Linear Eddy Model
Srinivasan, Menon, FlowTurb Comb 94, 237, Sankaran, Menon, PROCI 30, 575

11

Motivation: DNS examples (at low Reynolds numbers)

R. Sankaran, E. Hawkes, Jackie Chen) & T. Lu, C. K. Law Premixed DNS PROCI 31, 1291



Bell, Day, Driscoll "corregated" premixed DNS PROCI 31, 1299

DNS flame in rectangular duct - L. Vervisch, A. Poludnenko,
Bunsen, V-flame, jet in cross-flow J.H. Chen
IC engine, Gas turbine, industrial burner:

RANS = KIVA (FSD/coherent flamelet), Fluent (empirical)

12

Importance of state relations

We could solve partial differential equations for every variable, but then we would need source terms for each. Instead use Schvab-Zeldovich approach:

Assume turbulent diffusivity of mass (D_T) equals that of momentum (ν_T) and that of heat (α_T)

- Premixed flames: solve only the differential equation for non-dimensional temperature, called reactedness (this is the energy eqn) and its variance
- Non-premixed flames: solve only the differential equations for mean mixture fraction (the Z equation) and its variance
- Then use **state relations** to compute mean values of ρ, T, Y_i and turbulent reaction rates, using:

$$\bar{Y}_{CO}\ (\bar{Z}, \overline{Z'^2}) = \int_0^1 Y_{CO}(Z)\ \ P(Z, \bar{Z}, \overline{Z'^2})\, dZ$$

- Where to get the state relations ? From equilibrium chemistry, or from strained flamelet (non-equil) chemistry – we will discuss

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Turbulent reaction rate $\overline{\dot{\omega}}$ - the biggest unknown

The conservation equation for time-averaged CO mass fraction is:

$$\bar{\rho}\,\tilde{u}\,\frac{d\tilde{Y}_{CO}}{dx} + \bar{\rho}\,\tilde{v}\,\frac{d\tilde{Y}_{CO}}{dy} = \bar{\rho}\,\alpha_T\,\frac{d^2\,\tilde{Y}_{CO}}{dy^2} + \overline{\dot{\omega}_{CO}}$$

kg/s/m³ CO produced = ?

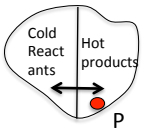
Turbulence-chemistry interaction – why do we need PDFs ?

Reaction rate depends on the JOINT PROBABILITY that:
sufficient fuel, sufficient O_2 and sufficient temperature are simultaneously present

You could ignore interactions and say the reaction rate is:

$$\overline{\dot{\omega}_{CO}} = \bar{Y}_{fuel}\ \bar{Y}_{O2}\ \exp(-E/R\bar{T})$$

That would be WRONG. Suppose a glob of pure reactants (cold) and a glob of pure products (hot) oscillate over point P, as shown:



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Why we need PDFs, continued

The actual temperature at P is 300 K when the reactants are present = no reaction

When products are present at P, temperature is 2100 K but no reactants = no reaction

If you use the time-average temperature at P, which is 2400/2 = 1200 K, and the time-average fuel-air ratio at P and plug into the above Arrhenius eqn, you compute a large reaction rate at P ! But reaction rate is nearly zero ! This is totally wrong.

Reaction occurs at P only when the thin line between the reactants and products is on P; then you have **simultaneously** the proper fuel, O_2 and temperature

The correct reaction rate of CO is the following, which has the PDF in it:

$$\overline{\dot{\omega}_{CO}}\left(\tilde{Z},\overline{Z''^2}\right) = \int_0^1 \dot{\omega}_{CO}(Z) \quad P\left(Z,\tilde{Z},\overline{Z''^2}\right) dZ$$

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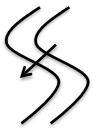
Turbulent reaction rate of a premixed flame - proportional to FSD

For a premixed turbulent flame, the turbulent reaction rate at any point, in kg/sec reactants consumed/volume, is needed because it is the source term in the mean conservation of energy equation. Reaction rate is given by:

$$\overline{\dot{\omega}_R} = \rho_R \; S_L \; \Sigma$$

Proof: Consider a wrinkled flame that at time t_1 moves normal to itself at speed S_L to new position at time t_2



The volume/sec of reactants overtaken by the wave = (area of wave A_T)
Times the (distance moved /sec) of each segment of the wave
distance moved / sec = S_L laminar burning velocity

mass/sec of reactants overtaken by the wave = ρ_R (volume/sec overtaken)
So: mass/sec of reactants overtaken = $\rho_R \, S_L \, A_T$

But: $\overline{\dot{\omega}}$ = mass/sec/volume = $\rho_R \, S_L \, (A_T/\text{volume}) = \rho_R \, S_L \, \Sigma$

See review of Driscoll, Prog Energy Comb Sci 34, 91

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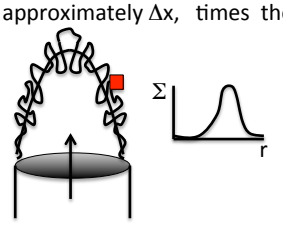
Premixed flame reaction rate depends on flame surface density

(FSD or Σ) = flame area per unit volume

$$\Sigma = \lim_{\Delta x \to 0} \frac{A_f}{(\Delta x)^3} = \lim_{\Delta x \to 0} \frac{P_f}{(\Delta x)^2}$$

A_f = average surface area of a premixed turbulent flame inside a small 1 mm^3 interrogation box

P_f = average perimeter of flame boundary inside a 1 mm^2 box in laser sheet
= average perimeter of flame when it is inside the box, which is approximately Δx, times the probability that it is inside box



FSD is a Gaussian-like function in space

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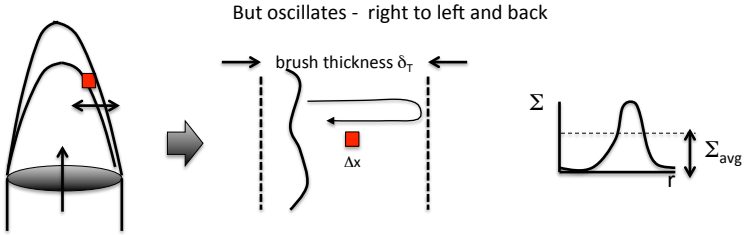
Physical meaning of FSD = flame surface density

Suppose flame is not wrinkled
But oscillates - right to left and back



a. perimeter of flame inside of interrogation box, when flame is inside box = approx. Δx

b. fraction of time flame is inside box is: $\Delta x / \delta_T$

Time avg perimeter in box is a x b = $(\Delta x)^2 / \delta_T$
Average FSD = avg perimeter / $(\Delta x)^2$ so:

Average FSD = approx. $1/\delta_T$ (= typically 0.2 mm^{-1})

FSD should be independent of box size Δx

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How to measure FSD ?

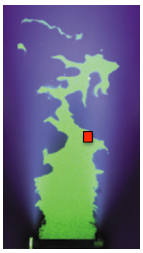


Image the flame boundary - using PLIF of OH or Mie scattering

Binarize the signal: green = 1, blue = 0

Canny edge detection - to obtain coordinates of a continuous contour, infinitely thin, fit to the flame boundary

Determine the average perimeter of this contour in the 1 mm^3 interrogation box; vary the box location

Resulting value of FSD must be independent of interrogation box size

Σ = [area of flame when it is in box) (prob. flame is in box] / $(\Delta x)^3$

Σ = approx. $[(\Delta x)^2 \ (\Delta x / \delta_T)]$ / $(\Delta x)^3$ so it should be independent of (Δx)

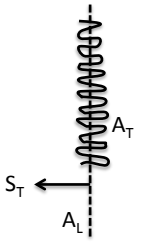
δ_T = brush thickness

31

Turbulence increases propagation speed - of a premixed flame

Damkohler first concept- moderate turbulence increases flame area by wrinkling

Consider this thin wrinkled flamelet; its wrinkled area is A_T, and the area of the straight dotted line is A_L



Each point on the wrinkled line propagates normal to the wrinkled line at a speed S_L, so the mass per second of reactants overtaken by the wrinkled line is $\rho_R S_L A_T$.

→ **So larger wrinkled area = more reactants consumed /sec**

The time-averaged wave is the dotted line; it propagates to left at S_T so the mass/sec of reactants dotted line overtakes = $\rho_R S_T A_L$

Equating these two mass flow rates, we get:

$$\frac{S_T}{S_L} = \frac{A_T}{A_L}$$

Turbulent flames propagate faster because they have more wrinkled surface area to consume the reactants

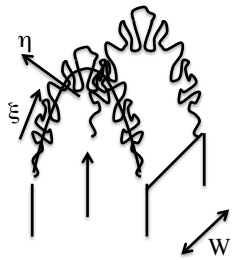
32

What is total wrinkled flame area A_T ?

A_T = Wrinkled flame area = area/volume integrated over the entire volume of the flame brush

$$A_T = \int \Sigma \, dV = \iint \Sigma \, d\eta \, d\xi \, W$$

Area / volume; normal; tangential; to brush



First definition of turbulent burning velocity S_T

Bray: assumed that thin flamelets propagate at S_L normal to themselves

Contribution of turbulent burning velocity due to thin flamelets is:

$$S_{T,F} / S_L = A_T / A_L$$

Where:

$$A_T = \int \Sigma \, dV = \iint \Sigma \, d\eta \, d\xi \, W$$

And $A_L = W\,L$ so:

$$S_{T,F} = S_L \, I_0 \, \frac{1}{L} \iint \Sigma \, d\eta \, d\xi$$

"flamelet contribution To turbulent burning Velocity" = total burning Velocity if in the thin Flamelet regime

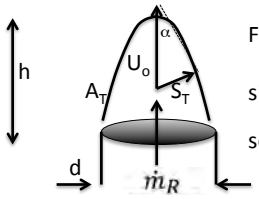
To measure $S_{T,F}$, measure Σ everywhere and integrate it over the flame brush

Second definition of turbulent burning velocity S_T

$S_{T,GC}$ = Global consumption speed

$S_{T,GC} = \frac{\dot{m}_R}{\rho_R A_T}$ = mass flow reactants / (density reactants) (area of $\bar{c}$ =0.5 surface)

How to measure $S_{T,GC}$?



From the triangle drawn:

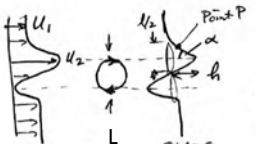
$\sin\alpha = [d/2]\ [h^2 + (d/2)^2]^{-1/2} = S_T/U_o$

so:

$$S_T = U_o\,(d/2)\,[h^2 + (d/2)^2]^{-1/2}$$

large burning velocity S_T = short flame

Damkohler's first concept - flame area A_T determines burning velocity



Imagine an eddy of diameter L moving at a stationary laminar flame at speed S_L; the eddy causes reactant to move at higher speed U_2 at one place, and at lower speed U_1 at another place

Suppose the flame wrinkles into two Bunsen cones, where α is the cone half-angle. Similar to a Bunsen burner, the velocity normal to the wave must be S_L, and the velocity normal to the cone is $(U_2\text{-}S_L)\sin\alpha$, so equating these gives:

$\sin\alpha = S_L / (U_2\text{-}S_L)$ and we define $u' = (U_2\text{-}S_L)$

the cone has a radius of L/4 and height h, so: $\sin\alpha = (L/4)[\,h^2 + (L/4)^2]^{-1/2}$

Equating these (and neglecting L/4 wrt h) yields: $h = (u'\,L)\ /\ (4\,S_L)$

Now the surface area of a cone is $A_T = \pi/4\,(L/2)^2\ [(h/(L/2))^2 + 1]^{1/2}$
and the area of the base of the cone is $A_L = \pi/4\,(L/2)^2$ so:

$$\frac{S_T}{S_L} = \frac{A_T}{A_L} = \left[1 + c_1 \left(\frac{u'}{S_L}\right)^2\right]^{1/2}$$

Predicted turbulent burning velocity
see Kuo, Turb Combustion

Damkohler's second concept - small eddies increase thermal diffusivity

$$S_L \sim \sqrt{\alpha\, RR}$$

$$S_T \sim \sqrt{(\alpha + \alpha_T)\; RR}$$

If eddies get inside preheat zone, we assume turbulent flames propagate faster because Eddies create larger thermal diffusivity α_T

$$\alpha_T = c_2\, u' L$$

turbulent diffusivity = velocity fluctuation times integral scale L; ν = kinematic viscosity

$$\frac{S_T}{S_L} = \sqrt{1 + c_2\, \frac{u' L}{\nu}} \quad \text{where} \quad \frac{u' L}{\nu} = Re_T$$

Turbulent flames propagate faster because turbulence diffuses the heat upstream to preheat the reactants faster than laminar flames

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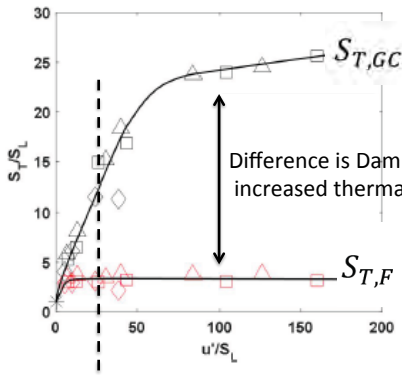
Turbulent burning velocity at "extreme" turbulence levels

Wabel, Skiba, Driscoll PROCI 36



$$S_{T,GC} = \frac{\dot{m}_R}{\rho_R\, A_T}$$

Global consumption speed

Difference is Damkohler second idea- increased thermal diffusivity

$$S_{T,F} = S_L\; I_0\; \frac{1}{L} \iint \Sigma\; d\eta\; d\xi$$

Contribution from Flame surface density (wrinkling)

previous turbulence levels

extreme turbulence levels

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Turbulent burning velocity – what do we know ?

1. Six major canonical geometries for premixed turbulent flames
   Bunsen, jet, low-swirl, V, spherical and swirl (Gas Turbine)
2. Burning velocity formula is different for each
3. Residence time (x/U) is important, bunsen flame tip becomes more wrinkled than flame base, spherical flame gets more wrinkled in time
4. Reactant temperature, Reynolds number , Karlovitz number are important
5. Role of integral scale different for each geometry - can we correlate burning velocity with Reynolds number Re_T ?

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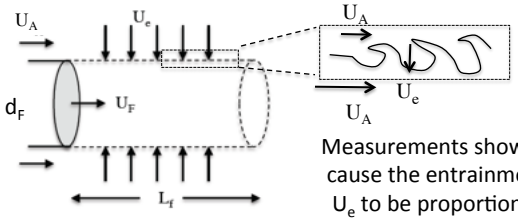
Turbulence Causes Faster Mixing = shorter flame length

Consider a non-premixed turbulent jet flame. Suppose we simplify by saying the fuel from the fuel tube - stays within the cylinder shown
Air enters at an entrainment velocity U_e that is perpendicular to the cylinder wall



(H. Rehab, J Fluid Mech 345, 357)

Measurements show that the eddies rotate to cause the entrainment velocity U_e to be proportional to $|c_1 U_F - U_A| (\rho_F/\rho_A)^{1/2}$

The length of the flame L_f is where the mass/sec of fuel, divided by the mass/sec of entrained air, equals the stoichiometric fuel-air ratio f_s, which is 0.055 for methane

$$\rho_F U_F \left(\pi \frac{d_F^2}{4}\right) / \left(\rho_A U_e \pi d_F L_f\right) = f_s$$

40

Laser Diagnostics used in Turbulent Combustion

AE 633 W17

Diagnostics: Raman (& line Raman), CARS (& line CARS), PLIF (LDV), Rayeigh, Stereo PIV

Non-premixed combustion

1.	Species mass fractions (Y_i)	
	Major species	**Raman** single point in blue (non-sooty) flames – methane, dimethyl ether (DME), CO2, H2O, CO, O2, N2
		Line CARS: fuel, CO2, H2O, CO, O2, N2
	Minor species	**PLIF:** of OH, formaldehyde CH2O, acetone tracer, CO, NO, NO2, JP-8, toluene, CH, O, H, HCO, iodine tracer
		Line CARS: ethane, propene during JP-8 pyrolsis
2.	Mixture fraction (Z)	Raman single point – in blue flames, from $CH_4 + H_2O$
3.	Scalar dissipation rate (χ)	**Line Raman** – Z at several points along a line
4.	Temperature	**Rayleigh** scattering, **CARS**, (thermocouples)
5.	Velocity field, Reynolds stress, k, integral scale, D_T, mixing rates, recirculation/separation zones	**Stereo PIV**, at 1 Hz or at kHz framing rates

Premixed combustion

6.	Reaction rates (ω)	PLIF of formaldehyde-OH overlap, or CH PLIF
7.	Reactedness (c)	Rayleigh or CARS for non-dimensional temperature
8.	Flame surface density (Σ)	OH or CH flame boundary inside small interrogation box
9.	Turbulent Burning Velocity (S_T)	OH or CH PLIF or Rayleigh images define flame boundary

Partially-premixed combustion

10.	Local fuel-air ratio	Raman single point
11.	Flame Index	PLIF of fuel and O2 gradients; aligned = premixed

Some questions to be answered using diagnostics

Non-premixed flames:

a) Assess models - by comparing profiles of mixture fraction, temperature, Y_i, dissip rate
b) What model is best ? one best in flamelet regime, one best in distributed regime ?
c) We cannot include hundreds of reactions in models; how many are needed ?
d) Do models work for different fuel types ? hydrogen/CO ? vaporized JP-8 ?
e) Measure scaling formulas: for flame length, D_T, dissip rate, with coflow air, swirl
f) Where are the internal recirculation or separation zones, how steady are they ?
g) Mixing and flameout limits: how does a recirculation zone (due to swirl) help ?
h) Where are CO, NO and soot produced in a flame ? from PLIF of Y_{CO}, $Y_{NO,}$ Y_{O2}, T
i) Do simplified soot models work ? When will a soot model work ?
j) Advantages of pulsed on-off fueling, effect of rapid fuel rise in emergency

Premixed flames

k) Flame surface density – compare measurements to models to determine best model
l) What new things happen at very high turbulence levels, typical of engines ?
m) Regimes ? Are the flamelets thin or broadened or broken ? or non-flamelet (distributed) ?
n) What factors promote distributed combustion: preheat, strong recirculation, low ig temp fuel
o) Does increasing turbulence continue to increase burning velocity (S_T) indefinitely ?
p) What is role of increased integral scale (large eddies) ?
q) How to stabilize a flame in a really high speed scramjet (supersonic) air flow ? (Flameout)
r) What is the combustion efficiency in a high speed scramjet ? Some fuel is not burned.
s) Mixing in cool air keeps temperatures down for cooler walls, low NOx, but causes extinction

Gas turbine-like Partially-Premixed flames

t) Assess the low NOx strategies of: RBQQ, LPP, EGR, air staging, ammonia reburn
u) Where are high temperature zones (T >1700 K) that produce NO, how to eliminate them ?
v) What are the residence times in complex recirculating flow that determine NOx, CO levels ?
w) Where is the fuel burning in non-premixed mode, where is it burning premixed ?
x) What is the local fuel-air ratio ?
y) Premixed flames often "growl" – acoustic instability because they are not properly anchored
kHz flame surface density, air velocity for spectra, phase angles to assess instability models
z) Measure local velocity at which flashback or blowout limits occur
aa) Prevent excessive heat transfer to dome, liner – where is cooling air going ?

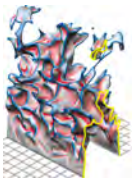
Tuesday: Kilohertz PLIF, PIV measurements

Turbulent Combustion

Experiments and Fundamental Models

J. F. Driscoll, University of Michigan

R. Sankaran, 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

Outline for Tuesday

1. **Canonical experiments**
2. **PLIF and KHz PLIF** - **of reaction layer structure –** Borghi regime diagram
3. **Kilohertz PIV movies of vorticity** - flame-eddy interactions
4. **Kilohertz PLIF** - movies of flame surface density to assess models of combustion instabilities, spectra, phase angles

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Canonical Non-premixed flames

1. Turbulent Jet flame (Sandia Flame D)
2. Jet in Co-Flow (Cabra burner)
3. Jet in Cross flow (JICF)
4. Gaseous Fuel Jet Surrounded by Swirling Air = Gas Turbine-Like
5. Spray flame – surrounded by swirling air = Gas Turbine-Like

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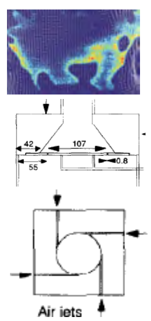
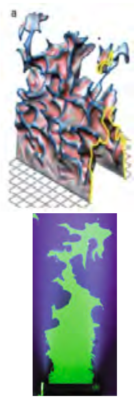
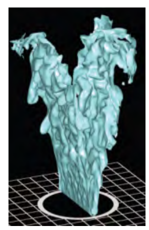
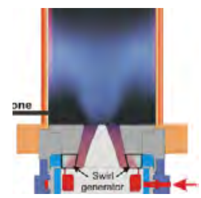
Canonical premixed turbulent flames

Low swirl	**Slot Bunsen**	**V-Flame**	**Piloted jet flame**	**Premixed Gas Turbine-like Swirl flame**
RK Cheng PROCI 31 3155	Driscoll, Bell PROCI 31, 1299	Gulder Comb Flame 162, 1422	Dunn, Masri Flow Turb Comb 85, 621	Meier, DLR Precinsta burner Comb Flame 150, 2







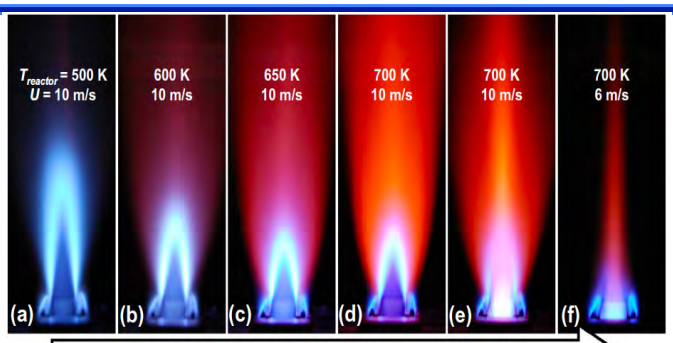


"Canonical premixed flames" - have been modeled

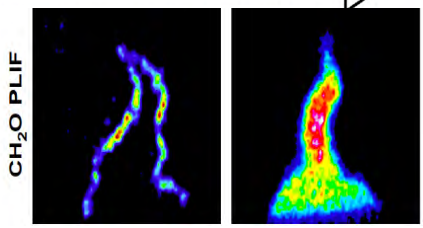
	type	experiments			DNS	LES	
1	low swirl	Berkeley	Cheng Shepherd	PIV, OH		Strakey, Pitsch	ThckFlm, G-eqn
2	low swirl	Lund	Alden Dreizler	PIV, T		Bai, Fureby	G-eqn, PaSR
3	2-D Slot Bunsen	Michigan	Driscoll Steinberg	PIV, CH	Grcar, Day		
4	2-D Slot Bunsen	none	(highly preheated)	none	JH Chen		
5	V-flame	Berkeley	Cheng Shepherd	PIV, T	Grcar, Day	Duwig	flamelet
6	V-flame	Hannover	Dinkelacker	PIV, T	Swamin.		
7	Bluff Body	FOI/Volvo	Volvo/Fureby	OH		Fureby	PaSR
8	jet, shear	Sydney	Dunn Masri	Raman,q			
9	jet, shear	Lund	Alden	CH, OH		Bai, Fureby	G-eqn, PaSR
10	jet, shear	Aachen	YC Chen, Peters	LDV,Raman		Pitsch	G-eqn
11	high swirl, gas t.	Darmstadt	Dreizler	PIV, Raman		Janicka	G-eqn
12	high swirl, gas t.	Karlsruhe	Siemens, PPC	LDV		Poinsot	ThickFlm
13	high swirl, gas t.	GE LM6000	Mongia, PPC			Menon, Fureby	LEM, PaSR

Ex.: Bunsen with Preheated reactants:

Yiguang Ju, SH Won, B Windom, B Jiang, Princeton U.



four regimes:
chemically-frozen-flow,
low-temperature-ignition,
transitional, and
high-temperature-ignition



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Diagnostics: Laser sheet imaging - of flame structure

Mie scattering – oil drops are in reactants but not products

Rayleigh scattering – temperature field = cold in reactants, hot in products

PIV – velocity field imaging – abrupt change at flame front

OH PLIF - uniform OH in products, no OH in reactants

CH PLIF - thin layer marks chemical reaction layer

Formaldehyde PLIF - marks preheat zone

OH-Formaldehyde overlap – thin layer that marks reaction layer

Raman scattering - primarily a point measurement, will work along a 2 mm line but not for imaging

CARS - primarily a point measurement will work along a 2 mm line, but not for imaging

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Mie and Rayleigh scattering

Mie – commercial kerosene oil drop atomizer adds 10 micron drops that evaporate at flame boundary, illuminate with any color laser sheet

Rayleigh - any color laser sheet, record with intensified camera light scattered from molecules

- must eliminate any dust or soot
- must eliminate any scattering off walls, windows

$$S_{Rayleigh} = [n_{N2}\,\sigma_{N2} + n_{fuel}\,\sigma_{fuel} + n_{O2}\,\sigma_{O2} + n_{CO2}\,\sigma_{CO2} + n_{H2O}\,\sigma_{H2O}]\; I_{laser}\; constant$$

where S = signal, n is number density and σ is Rayleigh scattering cross section. If a fuel is chosen that has the same cross section as N_2, then, approximately, all cross sections are nearly equal so:

$$S_{Rayleigh} = n\;\sigma_{N2}\;I_{laser} = \left[\frac{p}{RT}\right]\sigma_{N2}\;I_{laser}$$

Rayleigh signal is a measure of gas temperature

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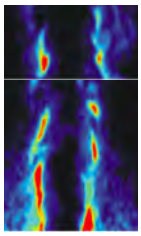
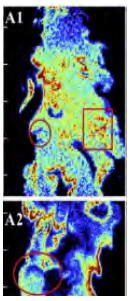
Challenge - two ways to image reaction zones

OH and formal-dehyde overlap



Dunn, Masri Bilger, Barlow
Flow, Turb. 85
(broken)

CH PLIF



Alden, Bai, Bo Zhou, Lund
PROCI 35
(distributed)

CH PLIF

Mastorakos, Meier, Gas Turbine Model Combustor (flamelet)

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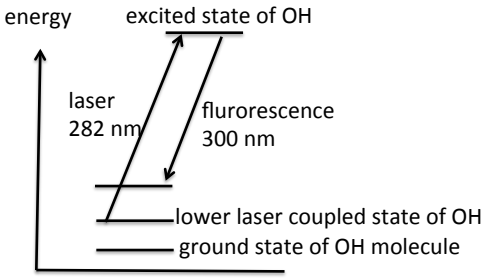
PLIF = planar laser induced fluorescence

Fluorescence = (absorption of laser light) + (spontaneous emission of light at a longer wavelength than the laser light)

OH absorbs laser light at 282 nm (in UV), emits fluorescence at 300-400 nm

Species that fluoresce
OH 282 nm
CH 390 nm
Formaldehyde 355 nm
NO 226 nm
NO_2 430 nm
Acetone 266 nm
Gasoline 270 nm
CO 230 nm
Iodine 514 nm
Ammonia 2000 nm
O 113 nm



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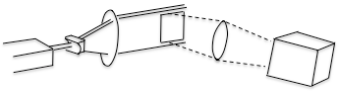
PLIF = planar laser induced fluorescence



Rate of molecules Excited to excited State by absorption = Rate of molecules Lost from excited state by spontaneous emission + Rate of molecules lost from excited state by collisional quenching

$$I_\nu \; n_{OH} \; f \; B_{12} = n^*_{OH} \; A_{21} + n^*_{OH} \; Q \quad (1)$$

n_{OH} = number density OH
B_{12} = absorption const.
A_{21} = emission const.
Q = quenching factor
c_1 = a constant
I_ν = laser intensity

Define signal from OH as: $S_{OH} = n^*_{OH} \; A_{21} \; c_1$ (2)

Solve Eq. (1) for n_{OH}* and plug into Eq. (2) to get:

$$S_{OH} = I_\nu \; [n_{OH} \; f] \; V \; B_{12} \; c_1 \; A_{21} \; (A_{21} + Q)^{-1}$$

Signal = laser intensity * number density of OH molecules in lower laser coupled state

f = Boltzmann fraction

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PLIF signal

Mole fraction of OH: $X_{OH} = n_{OH} / n$ total number density: $n = p/(k\,T)$

Laser volume $V = \Delta x^2\ \delta_{laser}$

$$S_{OH} = X_{OH} * \left[\frac{p}{T}\ E_L\ \frac{(\Delta x)^2}{H}\right]\left[\frac{f\,A_{21}}{Q+A_{21}}\right]\frac{const}{(FN)^2}$$

- S_{OH}: OH PLIF signal per camera pixel
- X_{OH}: OH mole fraction
- E_L: laser energy per pulse
- $(\Delta x)^2/H$: pixel size^2/ height of field of view
- $(FN)^2$: lens f-number^2

To maximize fluorescence signal S_{OH}, you can:

bin the pixels and make pixel size Δx larger, but you lose spatial resolution
reduce the height (H) of the field of view – more energy/volume of laser sheet
use small FN lens = larger diameter lens, FN = lens focal length / diameter of lens
increase laser energy per pulse E_L
increase gas pressure p

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Some limitations to PLIF diagnostics

The molecule of interest must absorb at a frequency of an available laser

(Water, CO_2, O_2, N_2, H_2 do not fluoresce, H and O are very difficult to fluoresce)

Molecule must emit fluorescence in visible or near UV or near IR where we have cameras

Fluorescence wavelength must be separated from fluorescence from other species

Difficult to get quantitative values of mole fraction – must measure quenching factor Q

Flame or soot radiation may create excessive background noise, esp. at high pressure

Must have sufficiently large windows to collect sufficient emitted light

Window glass can fluoresce and cause background noise

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Good references on fluorescence diagnostics

Hanson, RK, J. M. Seitzman, P. Paul, Planar Laser-Fluorescence Imaging of Combustion Gases, Appl. Phys. B 50, 441454 (1990)

Ekbreth, A., Laser Diagnostics for Combustion Temperature and Species, Combustion Science & Technology Pub.

Johnson, Raynor Carey. An introduction to molecular spectra

Herzberg, G. Spectra of Diatomic Molecules, Van Nostrand, 1950.

Ayoola B, Balachandran R, Frank J, Mastorakos E. Spatially resolved heat release measurements in turbulent flames. Comb. Flame 2006; 144: 1-16.

Marcus Alden, Xue-Song, Bai, Bo Zhou, Lund U., Comb. Flame 162, 2937, 2015

Wolfgang Meier, Adam Steinberg, et al. (kilohertz), Comb. Flame 157, 2250

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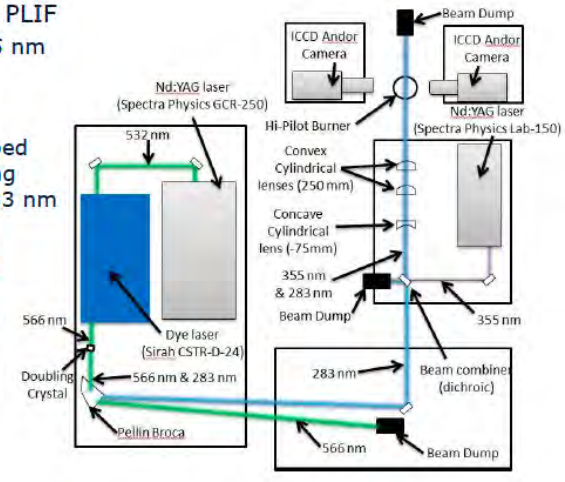
OH, Formaldehyde and CH PLIF diagnostics

- Formaldehyde (CH_2O) PLIF
  - Nd:YAG outputs 355 nm
- OH PLIF
  - Sirah dye laser pumped with 532 nm, doubling crystal produces ~283 nm
- Andor intensified CCD cameras
  - 100 ns gate times
  - 200 ns delay
  - 27 x 36 mm and 13 x 20 mm FOV



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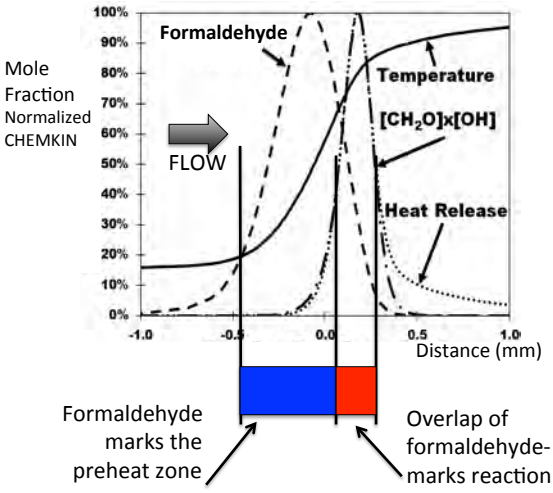
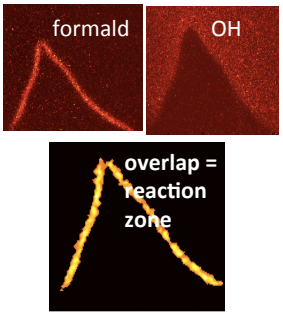
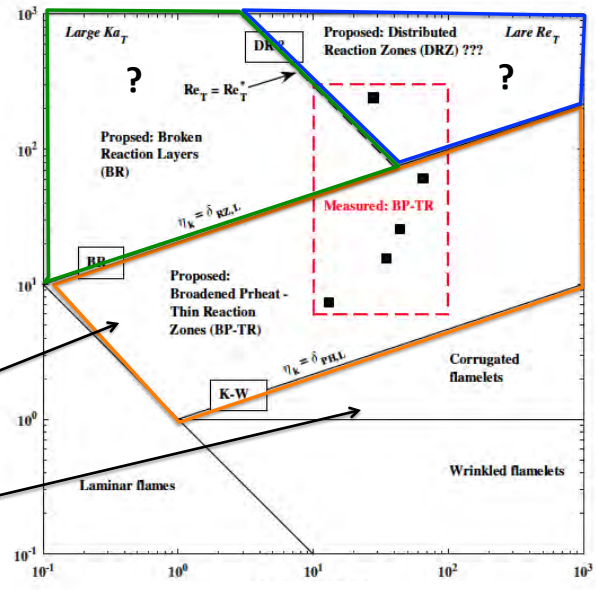
Reaction zone imaged with formaldehyde-OH overlap





Laminar bunsen flame

Regimes of Premixed Turbulent Combustion (Borghi diagram)



Turbulence Level u'/S_L

Damkohler's second concept

Damkohler's first concept

Integral scale, normalized by flame thickness

Regime boundaries

Klimov-Williams boundary is where $\delta_{PH} = \eta_K$

= where Kolmogorov eddies of size (η_K) fit inside the PREHEAT layer (δ_{PH}) of the flame

They predict: **"BP-TR" = Broadened preheat, thin reaction layers**

Define: Ka = Karlovitz number (Peters) = $(\delta_{RZ} / \eta_K)^2$

so if Ka > 1, Kolmogorov eddies of size (η_K) fit inside reaction zone (δ_{RZ}) of the flame

Peter's predicts Ka > 1 causes **"broken reaction layers"**

Are tiny Kolmogorov eddies strong enough to cause broken layers ? (NO)

We need to know these boundaries because:

they tell us conditions when the following models are valid or not: the FSD/ thin flamelet model,the TM = thickened flamelet model, DM = distributed reaction models

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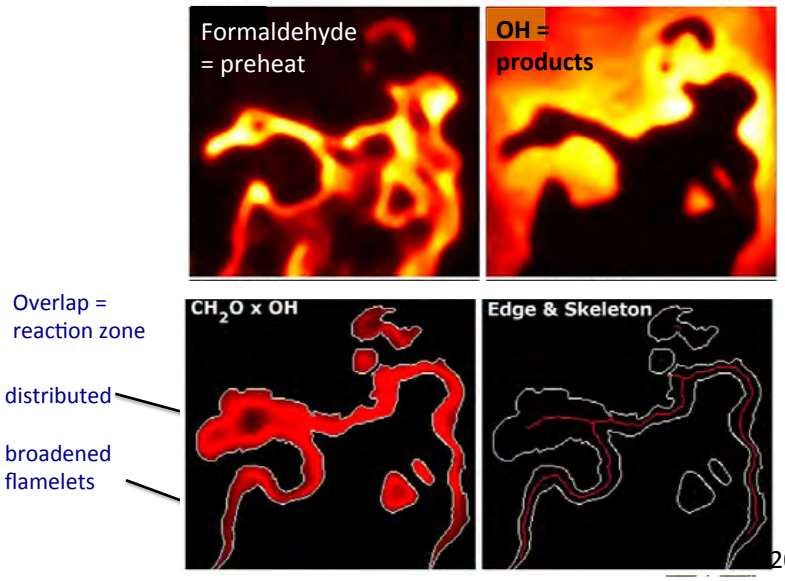
Reaction layers, Method #1: formaldehyde - OH overlap



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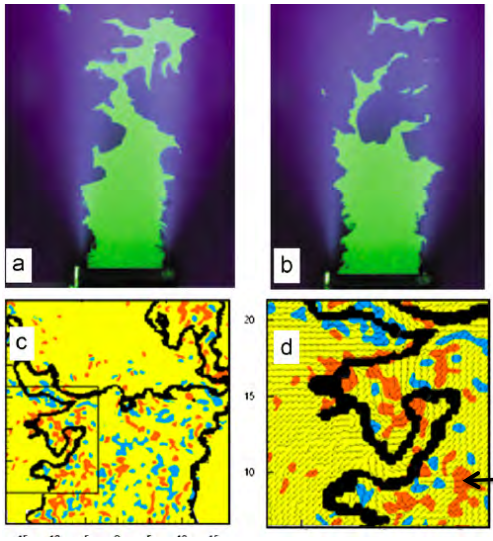
Reaction layers, Method #2: CH PLIF



Simultaneous CH – PIV
Carter and Driscoll
Comb Flame

← Reaction Layer
= CH PLIF

Vorticity =
eddies

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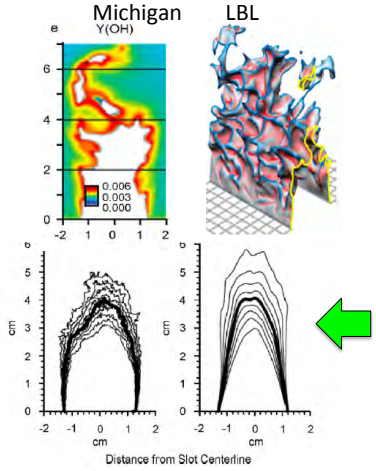
Assess DNS - of Bell (LBL) with experiment of Driscoll, Carter

Experiment
Driscoll,
Michigan

DNS
Bell,
LBL



DNS of Bell predicts a height
of slot bunsen flam, that agrees with the
experiment of Driscoll and Carter, thus
DNS yields the measured value of
turbulent burning velocity

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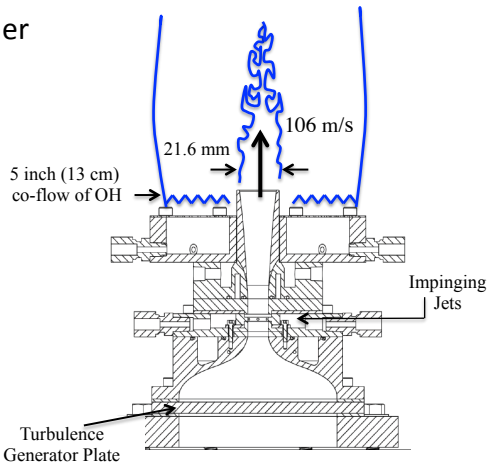
What happens as turbulence level is greatly increased ?
Do reaction layers become broadened, broken, distributed ?

Michigan Hi-Pilot Burner

- u'/S_L up to 243
- mean velocity to 78 m/s
- Re_t up to 100,000
- (preheat up to 1000 K)
- Methane, Butane, JP-8 at ER = 0.75, 1.05



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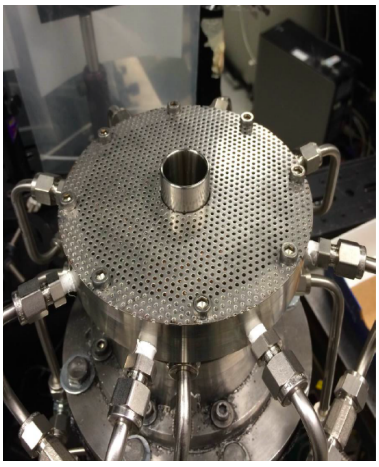
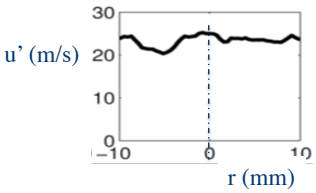
Hot co-flow of combustion products –
prevents outside air from being entrained



Turbulence is uniform
across burner exit



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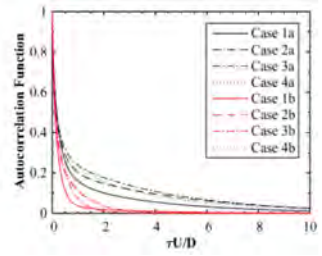
Turbulence levels and integral scales are large

Case	ϕ	U_0 (m/s)	u' (m/s)	λ_I (mm)	Re_T	Da_T	Ka_T	u'/S_L	$\lambda/\delta_{PH,L}$
2a	1.05	14	2.9	7.5	1,400	25.4	4.7	7.5	31
3a	1.05	32	6.0	20	7,900	33.1	8.5	15	84
4a	1.05	44	10	25	17,000	24.6	16.5	26	105
5a	1.05	64	24	37	58,000	15.1	50.4	62	154
6a	0.65	78	37	41	99,000	1.7	503	243	83



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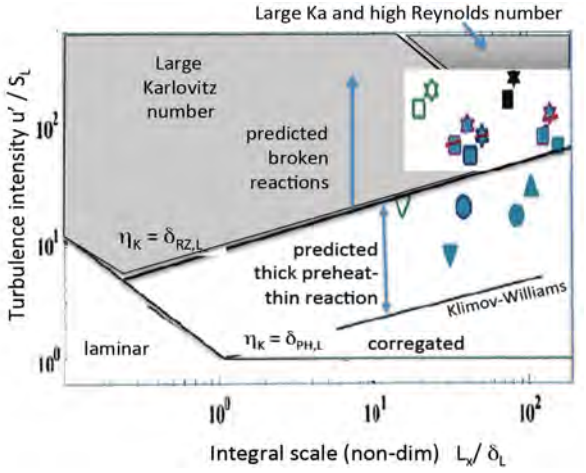
Hi-Pilot Conditions on Borghi Plot



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Hi-Pilot Burner

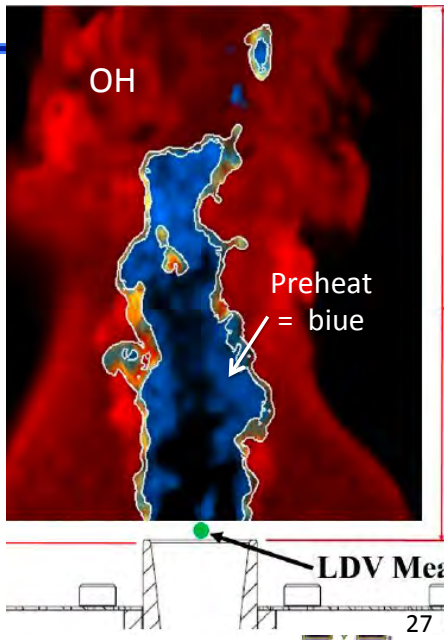
Thickness of Reaction zone

Thickness of Preheat zone

Fraction that is distributed

Fraction of local extinction

Boundaries of regimes



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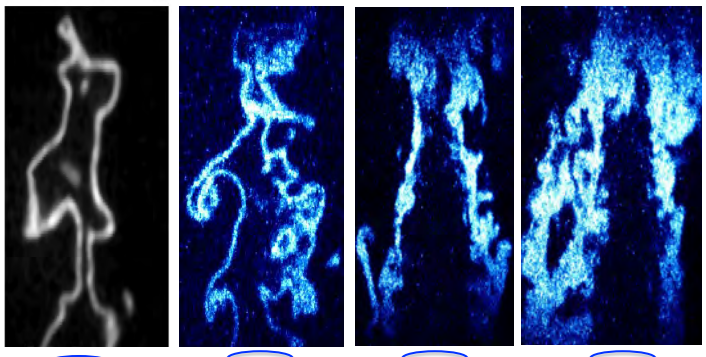
Preheat zone – what does it look like ? formaldehyde



u'/S_L = 3.0 7.5 26 62

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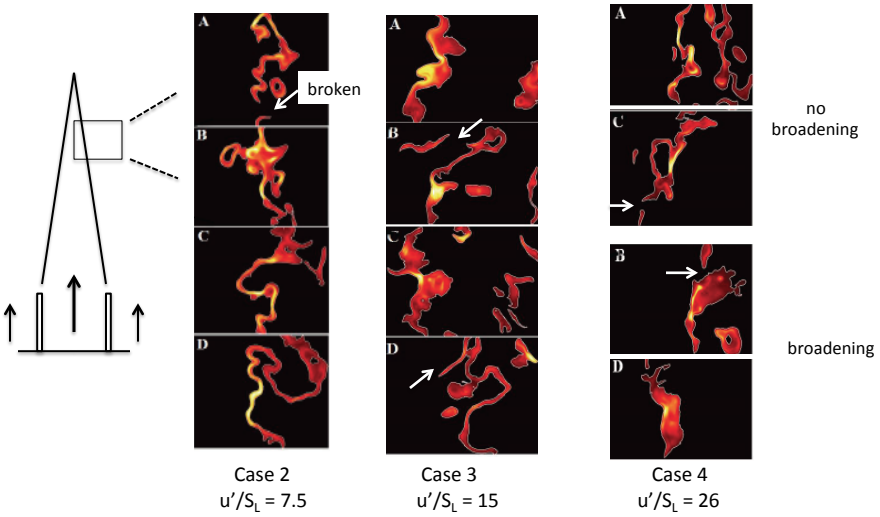
Reaction Layers (from overlap method)



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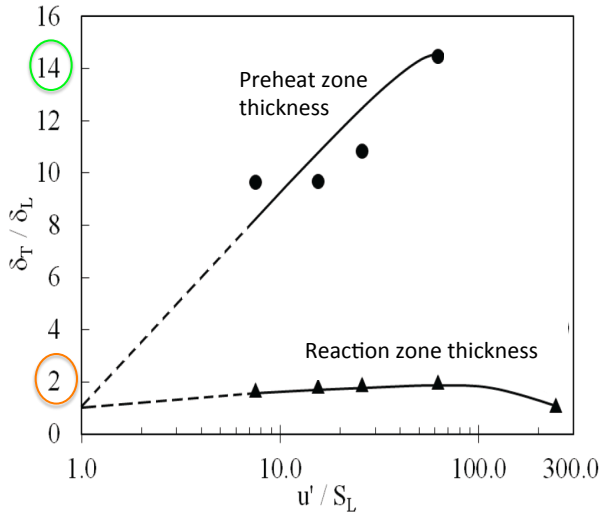
Preheat Zone is Thickened - Reaction Zone is not



$\delta_{PH,L}$ = 0.35 mm
$\delta_{RZ,L}$ = 0.18 mm

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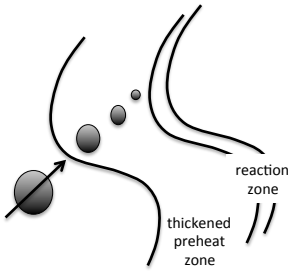
Preheat is 14 X broader, reaction zone only 2 X broader

thickening of preheat zones → eddies travel long distance through hot, viscous, preheat gases → eddies too weak to thicken reaction zone

↓

do larger integral scale eddies survive passage ?



Stretch Efficiency Function - Poinsot

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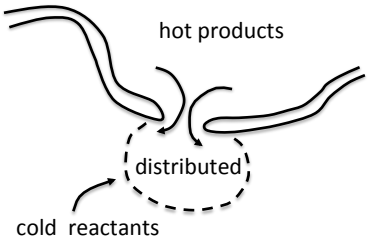
Are "broken" and "distributed" regimes related ?

broken - flamelets allows reactants to mix with products, promotes:

distributed - reactions ?



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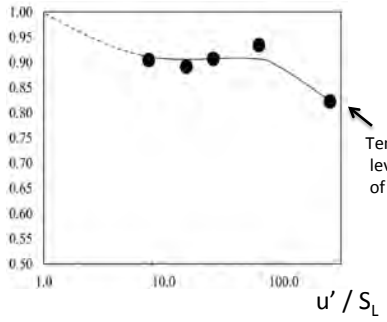
Burning fraction - always above 82% for homogeneous products

Burning Fraction

fraction of OH boundary that has reaction



Ten times the turbulence level of previous studies of this type

→ "broken regime" - is not possible if products are kept homogeneous and hot

"broken regime" IS possible if products are stratified (for this expt.)

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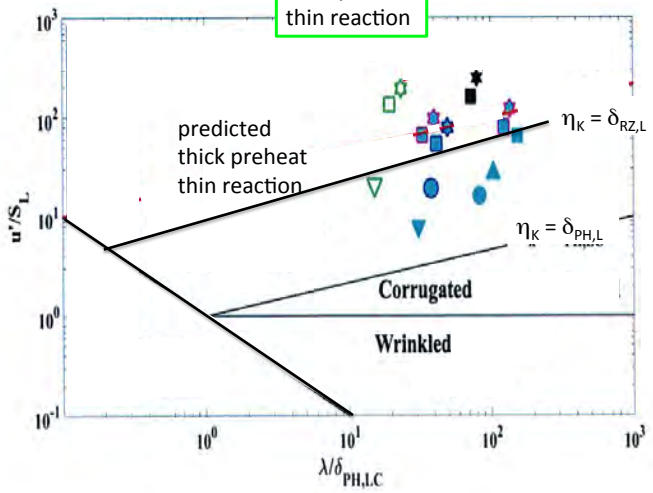
Measured thick preheat/thin reaction zone is larger than predicted

measured thick preheat thin reaction



predicted to be broken but are not broken

Peters boundary does not agree with our measurements

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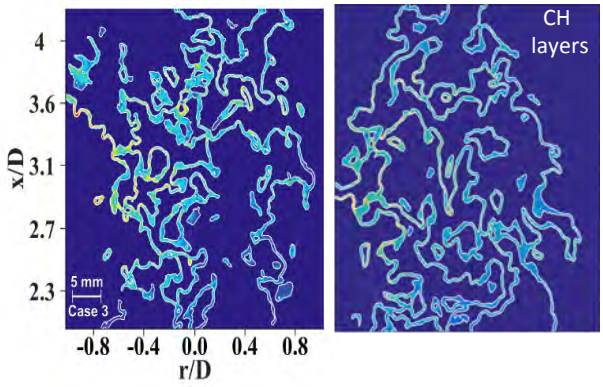
Densely Packed Flamelets - Regime



If flamelets are this densely-packed – can we model them as "distributed reactions" ?

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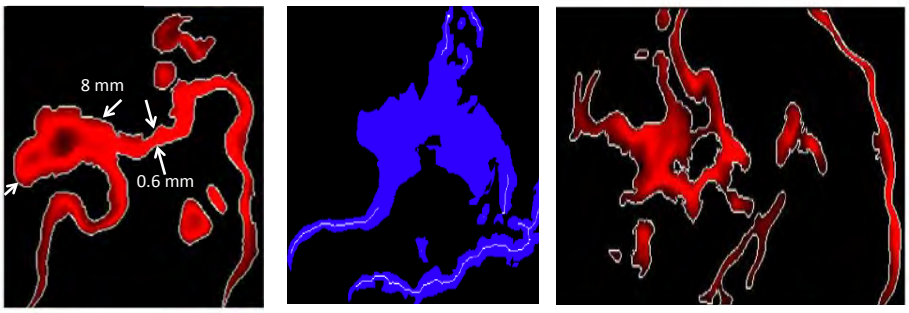
"Partially-distributed" regime

10 % of OH boundary has distributed reactions for highest turbulence



see: "blobs of chicken in a noodle soup"

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