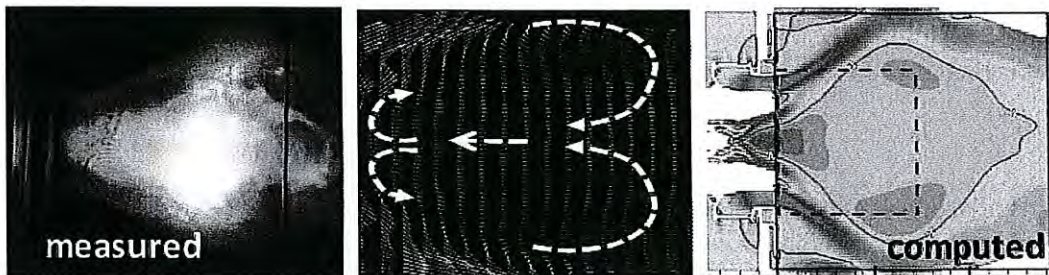


Advanced (Turbulent) Combustion

Aerospace Engineering 633

Winter Term 2017, J. F. Driscoll, instructor

Monday and Wednesday 3:00 – 4:30 pm, Room 1012 FXB



Lean Premixed Prevaporized Combustion in our GE TAPS Gas Turbine Combustor

Course Outline by week:

- 1 Theory of Strained Non Premixed Flamelets
- 2,3 General concepts of turbulence applied to combustion
- 4,5,6 Non-premixed turbulent combustion – modern models and experiments
- 7 Theory of Flame Stretch - of premixed flamelets
- 8,9 Premixed turbulent combustion – modern models and experiments
- 10,11 Modern laser imaging diagnostics applied to turbulent combustion
- 12,13 Partially-premixed combustion and flame blowout theory

Note: We will not do any programming in this course. Instead we will run FLUENT tutorials (that are carefully documented) for RANS and LES cases.

Aerospace Engineering 633

Turbulent Combustion

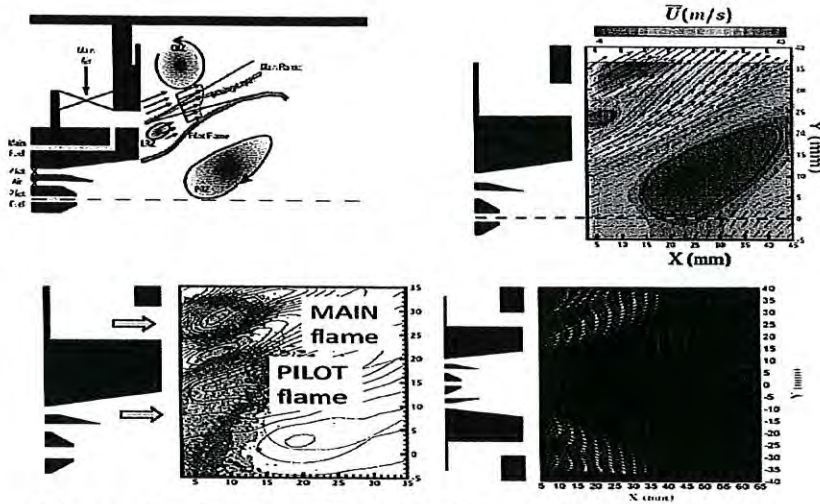
Winter Term 2017, J. F. Driscoll, instructor

Times and Location: Mon and Wed: 3:00 – 4:30 pm, Room 1012 FXB
Prerequisites: AE 533 Combustion or equiv.; AE 525 Turbulence is not required
Instructor: James F. Driscoll, 3004 FXB, jamesfd@umich.edu, ph: 936-0101
Office Hours: Tues & Thurs 2:30 pm – 4:00 pm or by appointment
Grading: Two exams= 50%, no final, Homework = 50% due Fri 5 pm
Textbook: None. CANVAS contains chapters from these textbooks:
Kuo, K.K., Fund. Of Turbulent and MultiPhase Combustion, read only Chpts 1-6
Peters, Norbert, Turbulent Combustion \$146 new, \$112 used, Cambridge U. Press, 2000
Turns, S., An Intro to Combustion, McGraw Hill, 2000
Lewis, B. and von Elbe, G., Combust. Flames, Explosions, Academic Press, 1961

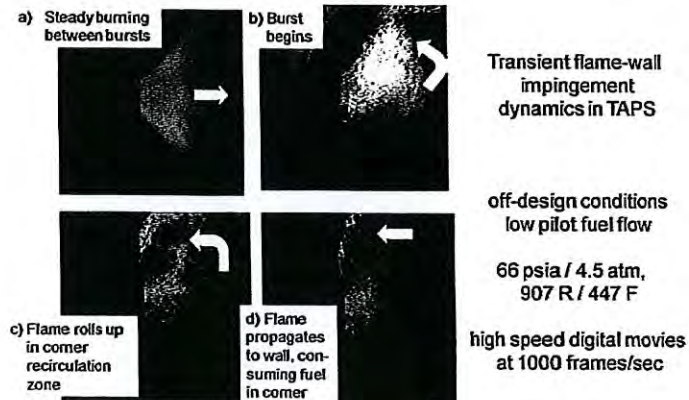
Week:

- 1 Theory of Strained Non Premixed Flamelets**
concepts of conserved scalar, scalar dissipation rate
- 2, 3 General concepts of turbulence applied to combustion**
assumed PDF shape, sub-models for dissipation rate
- 4, 5, 6 Non-premixed turbulent combustion – modern models and experiments**
 - a. simple RANS flamelet model of FLUENT
 - b. modern LES flamelet model of Pitsch, FPV model of Moin
 - c. non-flamelet modern models for distributed combustion
- 7 Theory of Flame Stretch - of premixed flamelets**
- 8, 9 Premixed turbulent combustion – modern models and experiments**
 - a. Flame surface density equation
 - b. CFM = Coherent Flamelet LES Model of Bray-Moss-Libby
 - c. G-equation LES model of Pitsch
- 10, 11 Modern laser imaging diagnostics applied to turbulent combustion**
- 12, 13 Partially-premixed combustion and flame blowout theory**
 - a. Modern PPC models of Pitsch, Vervisch
 - b. Theory of flame blowout in engines and scaling relations

TAPS Lean Premixed Prevaporized Fuel Injector for GEnx engines on Boeing 787 Dreamliner



Flame visualization Formaldehyde PLIF



Desired:

1. Low NOx: lean, uniformly low temperature field
2. Stable: flame anchored and steady, need: large turbulent burning velocity
3. Avoid flashback – burning velocity not too large
4. Avoid growl – no acoustic instability
5. Need “Design CFD Model” of turbulent combustion

Non-Premixed Turbulent Combustion Models

MODELS = Large Eddy Simulations (LES) of Non Premixed Turbulent Combustion

(a) flamelet LES models. - work for most problems but maybe not for distributed combustion, autoignition

- | | | | |
|---|---------------------------------------|----------------|---|
| 1 | SFL Steady Flamelet | Pitsch, FLUENT | simple, experimentally validated, does chemistry, not extinction not yet applied to partially premixed, |
| 2 | FPV Flamelet Progress Variable | Moin, Ihme | replace scalar dissipation rate with progress variable may work better with extinction and partially premixed |

(b) non-flamelet models. - much more costly but may work better for distributed comb., autoignition

- | | | | |
|---|--|-------------------|--|
| 3 | PDF PDF Transport | Pope, Raman | very expensive, many equations not experimentally validated does chemistry exactly but poor job of turb. and molec diffusion |
| 4 | DNS Direct Numerical Simulation | JH Chen, Vervisch | way of the future but limited to modest Reynolds number and reduced chemistry, simple geometries |

References:

SLF = Steady Laminar Flamelet, Strained, RANS – two scalar (f, χ)

1. FLUENT manual Chapter 15.3, The Laminar Flamelet Model
2. A W. Cook, J. Riley, G Koshaly A Laminar Flamelet Approach to Subgrid-Scale Chemistry in Turbulent Flows, Combust Flame 109:332-341 (1997)
3. A. Kempf, F. Flemming, J. Janicka, Investigation of length scales, scalar dissipation, and flame orientation in a piloted diffusion flame by LES, PROCI 30 (2005) 557–565.
4. Heinz Pitsch, Large-Eddy Simulation of Turbulent Combustion, Annual Rev. Fluid Mech. 2006, 38:453–82.
5. Riley, J., Review of LES of Non-Premixed Turbulent Combustion J. Fluids Engr. 128, 209, 2006
6. H. Pitsch, N. Peters, CNF 114 (1998)

FPV flamelet progress variable – best for extinction and PPC

7. M Ihme, H Pitsch, Prediction of extinction and reignition in nonpremixed turbulent flames using a flamelet progress variable model, Application in LES of Sandia flames D and E, Combust Flame 155 (2008) 90–107
8. M Ihme, YC See, Prediction of autoignition in a lifted methane/air flame using an unsteady flamelet/progress variable model, Combustion and Flame 157 (2010) 1850–1862
9. C D Pierce, P Moin, Progress-variable approach for large-eddy simulation of non-premixed turbulent combustion J. Fluid Mech. (2004), 504, 73–97.

PDF Transport

10. Pope, S.B., Prog Energy Com Sci 11, 119, 1985
11. J. Xu, S.B.Pope, PDF Calculations of Turbulent Nonpremixed Flames with Local Extinction, Combustion and Flame 123:281–307 (2000)
12. Q Tang, J Xu and S B. Pope, PDF Calculation of Local Extinction and NO Production in Piloted Jet Turbulent Methane Air Flames, Proc Combust Inst, 28, 2000, 133–139
13. M.R.H. Sheikhi, T.G. Drozda, P. Givi, F.A. Jaber, S.B. Pope, Large eddy simulation of a turbulent nonpremixed piloted methane jet flame, Proc Combust Inst 30 (2005) 549–556
14. Raman, V., H. Pitsch, and R. O. Fox (2006). Eulerian transported probability density function sub- filter model for large-eddy simulation of turbulent combustion. Combustion Theory and Modelling 10.(3), 439–

CMC Model – will not be covered in AE 633

15. M. R. Roomina, R. W. Bilger, Conditional Moment Closure (CMC) Predictions, Comb Flame 125:1176 (2001).

“Turbulence-Chemistry Interactions” are statistical in nature

$$\frac{\partial}{\partial x} (\bar{\rho} \bar{u} r \bar{Y}_{H_2}) + \frac{\partial}{\partial r} (\bar{\rho} \bar{v} r \bar{Y}_{H_2}) = \frac{\partial}{\partial r} \left(\bar{\rho} D r \frac{\partial}{\partial r} (\bar{Y}_{H_2}) \right) + \bar{\dot{\omega}}_{H_2}$$

How to model $\bar{\dot{\omega}}_{H_2}$? = kg/s/m³ of H₂ created = negative

Suppose we have H₂ + 1/2 O₂ → H₂O then Arrhenius says

$$\dot{\omega}_{H_2} \sim Y_{H_2} (Y_{O_2})^{1/2}$$

if you assume no turbulence chemistry interactions;

$$\bar{\dot{\omega}}_{H_2} \sim \bar{Y}_{H_2} (\bar{Y}_{O_2})^{1/2}$$

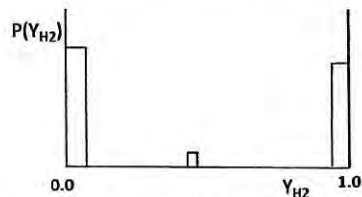
suppose you have thin non-premixed flamelets such that at a point P:

10% of the time the flamelet is on top of P, such that at that time: Y_{H₂} = 0.5 and Y_{O₂} = 0.5

40% of the time pure fuel is on top of P, so at that time Y_{H₂} = 1.0 and Y_{O₂} = 0.0

50% of the time pure O₂ is on top of P, so at that time Y_{H₂} = 0.0 and Y_{O₂} = 1.0

The PDF = probability density function = histogram of Y_{H₂} is:



$$\text{then: } \bar{Y}_{H_2} = 0.10 (0.5) + 0.40 (1.0) + 0.5 (0.0) = 0.45 = \int_0^1 Y_{H_2} P_{H_2} dY_{H_2}$$

$$\bar{Y}_{O_2} = 0.10 (0.5) + 0.50 (1.0) + 0.5 (0.0) = 0.55 = \int_0^1 Y_{O_2} P_{O_2} dY_{O_2}$$

$$\text{so } (\bar{Y}_{H_2} \bar{Y}_{H_2}) = 0.247$$

$$\text{But } (\overline{Y_{H_2} Y_{O_2}}) = 0.10 (0.5) (0.5) + 0 + 0 = 0.025$$

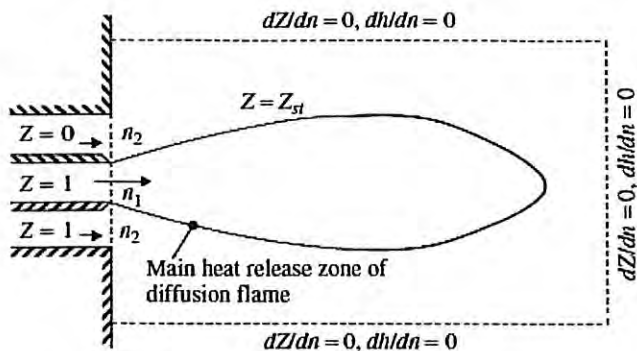
Conclude: you must know the joint probability that both fuel and oxidizer are present

This requires some knowledge of the structure of the chemical reaction region

(If you did not have thin flamelets, but distributed reactions such that everywhere you had a spatially uniform mass fraction of H₂ and a uniform mass fraction of O₂, then you could just multiply the mean values.)

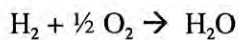
Non-Premixed Laminar Jet Flame (Kuo p. 131, see Canvas)

Fuel = H₂, oxidizer = O₂ at 300 K initially, subscripts i = 1,2 refer to x, r directions



$$\frac{\partial \rho u_i Y_F}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho D_F \frac{\partial Y_F}{\partial x_i} \right) + \dot{\omega}_F$$

$$\frac{\partial \rho u_i Y_{O_2}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho D_{O_2} \frac{\partial Y_{O_2}}{\partial x_i} \right) + \dot{\omega}_{O_2}$$



so 1/2 mole O₂ consumed for 1 mole H₂, so 16 g O₂ consumed for each 2 g of H₂,

since $\dot{\omega}_F$ is - (grams fuel consumed per second per unit volume), thus $\dot{\omega}_F = 1/8 \dot{\omega}_{O_2}$

Mixture Fraction (Z)

Define Z = mixture fraction based on hydrogen atoms

$$Z = (Y_H - Y_{H,2}) / (Y_{H,1} - Y_{H,2}) \quad \text{where:}$$

Y_H = mass fraction of hydrogen atoms, no matter what molecule they are in

Y_{H,1} = mass fraction of hydrogen atoms within fluid in stream 1 = 1

Y_{H,2} = mass fraction of hydrogen atoms within fluid in stream 2 = 0

Assume that: all diffusivities are the same (equal diffusivity, unity Lewis number)

fast chemistry = all reactions occur within the very thin black line drawn

Now multiply the second equations above by -1/8 and add it to the first equation

The source term in the resulting equation becomes ($\dot{\omega}_F - 1/8 \dot{\omega}_{O_2}$) which is zero.

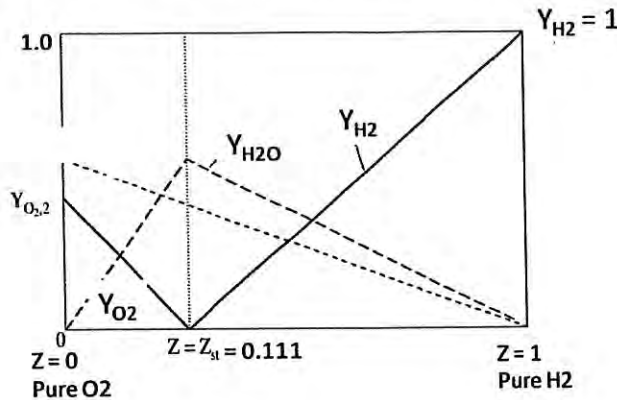
The other terms become:

$$\rho u_i \frac{\partial Z_j}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial Z_j}{\partial x_i} \right)$$

Kuo p. 131: mixture fraction conservation eqn.

State relations - for equilibrium (fast) chemistry

State relations are formulas for Y_{H_2} , Y_{O_2} , Y_{H_2O} , T , ρ as functions of Z alone - for fast chemistry (for realistic chemistry we will show they are functions of two variables, Z and χ_s , where χ_s is the stoichiometric scalar dissipation rate). Kuo, p. 134:



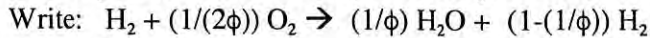
The vertical axis is mass fraction and the horizontal axis is mixture fraction (Z)
 $Z=0$ is pure O_2 , $Z=1$ at right side of graph is pure H_2 .

Assume: fast chemistry, H_2 and O_2 cannot co-exist except at thin flame front
 So any point outside flame front must be products and O_2 (no H_2)
 Any point inside the flame front must be products and H_2 (no O_2)

→ How to compute the state relations for hydrogen-oxygen fast chemistry:

1. First consider lean conditions outside the jet flame above, ϕ = local equivalence ratio
 Write: $H_2 + (1/(2\phi)) O_2 \rightarrow H_2O + \frac{1}{2} ((1/\phi)-1) O_2$
 For fast chemistry, fuel and oxidizer cannot co-exist except at the thin flame front,
 So the mixture at any point outside the flame is the mixture on right side (products & O_2)
2. For the two gases on the right side (water and O_2)
 - a) $Z = Y_H = 2 / (18 + \frac{1}{2} ((1/\phi)-1)32)$, since $Y_{H,1} = 1$ and $Y_{H,2} = 0$
 - b) $Y_{O_2} = \frac{1}{2} ((1/\phi)-1) 32 / (18 + \frac{1}{2} ((1/\phi)-1)32)$,
 - c) $Y_{H_2O} = 18 / (18 + \frac{1}{2} ((1/\phi)-1)32)$ and $Y_{H_2} = 0$
3. Simplifying:
 - a) $Z = \phi / (\phi+8)$, so plug in $\phi = 1$ to get $Z_s = 1/9 = 0.111$
 - b) Also the above simplify to:
 $Y_{O_2} = (8-8\phi)/(\phi+8)$,
 $Y_{H_2O} = 9\phi / (\phi+8)$, $Y_{H_2} = 0$
 $\phi = 8Z(1-Z)$
4. Solve eqn (3a) for ϕ to find:
5. Plug this into 3b to get:
 $Y_{O_2} = 1 - (Z/Z_s)$ $Y_{H_2O} = (Z/Z_s)$, $Y_{H_2} = 0$
 These are the three lines on the above plot to the right of $Z = 0.111$.

6. Now repeat for the rich side (inside the jet flame)



7. The actual gas mixture inside flame is water plus H_2 , so it is the right side of this eqn

a) $Z = Y_H = [(1/\phi) 2 + (1-(1/\phi)) 2] / [(1/\phi) 18 + (1-(1/\phi)) 2]$, and

b) $Y_{H_2} = (1-(1/\phi)) 2 / [(1/\phi) 18 + (1-(1/\phi)) 2]$

c) $Y_{H_2O} = (1/\phi) 18 / [(1/\phi) 18 + (1-(1/\phi)) 2]$ and $Y_{O_2} = 0$

8. Simplify this to:

$Z = \phi / (\phi+8)$ so $Z_s = 1/9$, $Y_{H_2} = (\phi - 1) / (\phi+8)$, $Y_{H_2O} = 9 / (\phi+8)$

9. Solve the first eqn for ϕ to get: $\phi = 8Z / (1-Z)$ and plug this into the other two eqns:

$Y_{H_2} = (Z - Z_s) / (1 - Z_s)$

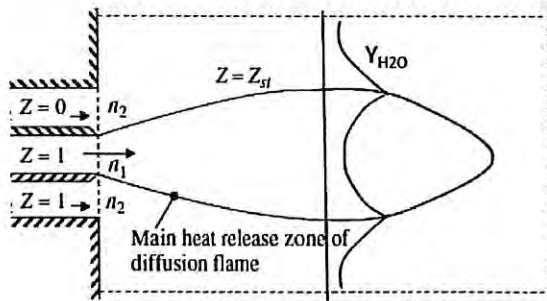
$Y_{H_2O} = (1 - Z) / (1 - Z_s)$ and $Y_{O_2} = 0$

These relations are the straight lines on graph to the left of $Z = 0.111$

Gas temperature: repeat above and compute the adiabatic flame temperature at each mixture fraction Z . The curve will reach a maximum at $Z = Z_s = 0.111$ and will be 300 K at $Z = 0$ (pure O_2) and at $Z = 1$ (pure fuel).

→ Conclude: for a laminar non premixed jet flame, at every point P in the flow field, I can

- solve the Z conservation equation above for Z and then
- use state relation graph to find the values of Y_{H_2} , Y_{O_2} , Y_{H_2O} , T , ρ at point P
- plot mass fractions, such as that of water vapor on the figure below:



Define:

A "conserved scalar" is a scalar quantity that has no source term in its conservation eqn.

Mixture fraction Z is a conserved scalar; Z varies in space due to convection and diffusion, so you must solve the Z eqn, but it has no nasty source terms that would have Arrhenius reaction rate factors in them that have exponential dependence on temperature. Another conserved scalar is enthalpy (we include both sensible and chemical enthalpy)

We can solve the following equations (see Kuo)

$$\frac{\partial}{\partial x}(\rho ur) + \frac{\partial}{\partial r}(\rho vr) = 0$$

$$\frac{\partial}{\partial x}(\rho ur Z) + \frac{\partial}{\partial r}(\rho vr Z) = \frac{\partial}{\partial r} \left(\rho D r \frac{\partial}{\partial r}(Z) \right)$$

$$\frac{\partial}{\partial x}(\rho ur u/U_0) + \frac{\partial}{\partial r}(\rho vr u/U_0) = \frac{\partial}{\partial r} \left(\mu r \frac{\partial}{\partial r}(u/U_0) \right)$$

$$\frac{\partial}{\partial x}(\rho ur h^*) + \frac{\partial}{\partial r}(\rho vr h^*) = \frac{\partial}{\partial r} \left(\rho \alpha r \frac{\partial}{\partial r}(h^*) \right)$$

h^* is a normalized enthalpy, which is $(h-h_2)/(h_1-h_2)$, so h^* is one in the jet which is fuel, and is zero in the coflow which is oxidizer

We assume that $\mu/\rho = D = \alpha$, so it follows that since u/U_0 , Z and h^* obey the same equations and have the same boundary conditions, then

$$u/U_0 = Z = h^* \quad \text{at each point } (x, r) \text{ in the jet}$$

So we only need to solve the Z equation to get Z , u/U_0 and h^*
(then solve continuity eqn for radial velocity v)

Laminar axisymmetric jet flame - see Kuo

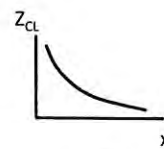
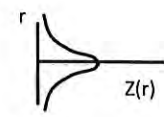
Kuo, K. Principles of Combustion

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

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

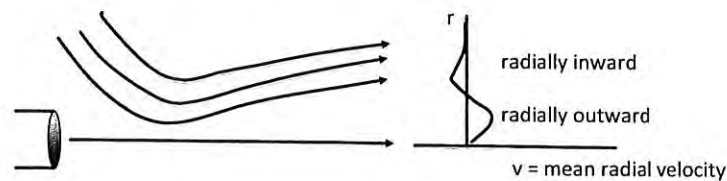
$$\xi = \left(\frac{r}{x} \right) \left(\frac{U_F d_F}{D} \right) \frac{\sqrt{3}}{8}$$

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



Mean radial velocity (v) - in simple jet model

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



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

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

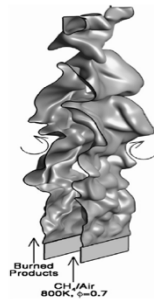


1-10

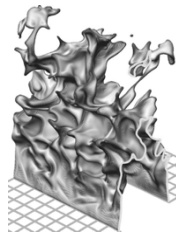
Turbulent Combustion

Experiments and Fundamental Models

J. F. Driscoll, University of Michigan



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



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

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1

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



2

Outline for Monday = Physical concepts

Motivation - premixed is the way of the future – low NO_x, CO, soot

What problems are important ?

Background what does turbulence do ?
what do we need to model and to measure ? turbulent
burning velocity, flame surface density, reaction rate

Turbulent reaction rate

Probability density function helps to model turbulent reaction rate

Fuel air mixing and Flame stability



3

Good references

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J. F. Driscoll, Turbulent premixed combustion: flamelet structure and turbulent burning velocities, Prog Energy Combust Sci 34, 91-134, 2008.



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

Eckbreth, Alan, Laser Diagnostics for Combustion Temperature and Species,
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Pitsch H, Large-eddy simulation of turbulent combustion, Ann Rev Fluid Mech 38, 2006

Duclos JM, Veynante D, Poinso 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.

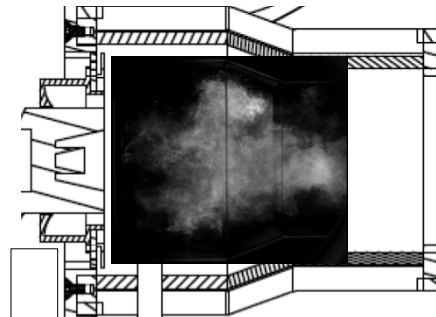
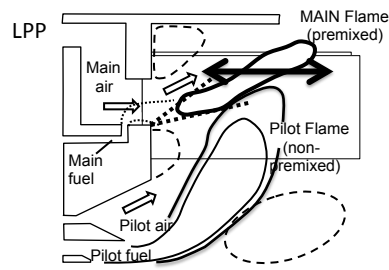
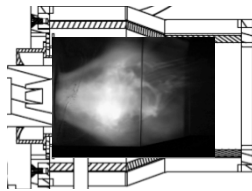
Kalghatgi, G.. Blowout stability limits of gaseous jet diffusion flames in still air,
 Combust Sci Technol 26, 233, 1981.



5

Motivation: Premixed is the way of the future - low NO_x, 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:** Poinot (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

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 ?

	<i>PREMIXED LES</i>	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
<i>NON PREMIXED LES</i>			
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, Poinot, 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

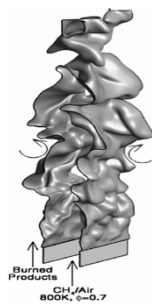
Knudsen, Pitsch, Comb Flame 159, 242, Nogenmyr, Comb Flame 156, 25

LEM = Linear Eddy Model

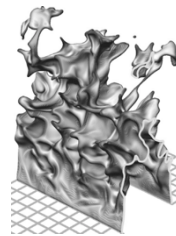
Srinivasan, Menon, FlowTurb Comb 94, 237, Sankaran, Menon, PROCI 30, 575

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
 "corrugated"
 premixed DNS
 PROCI 31, 1299

DNS

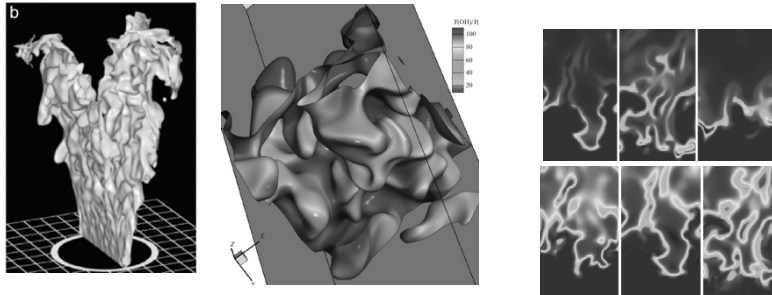
flame in rectangular duct - L. Vervisch, A. Poludnenko,
 Bunsen, V-flame, jet in cross-flow J.H. Chen
 IC engine, Gas turbine, industrial burner:

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



12

DNS - 3-D, complex chemistry



Bell, Proc Natl Acad Sciences 102, 29
10006–10011

Aspden J. Fluid Mech 680, 287
Flame in a duct – periodic boundary conditions
Sees broken reactions
Claims to see distributed reactions



13

Background – what does turbulence do ?

Faster mixing - large turbulent diffusivity, shorter flames, smaller combustors

Faster propagation - large turbulent burning velocity avoids blowout

Optimize liftoff height - keep flame away from walls but do not blowout

Reduce Pollutants - less NO_x if velocities are large (for short residence times)
and fuel-air mixing is fast and lean

Avoid growl - combustion oscillations in gas turbines, rockets, due to poor
flame anchoring

Challenge: to model the turbulent reaction rate for
non-premixed, premixed and partially-premixed combustion
what are the best current models, and how good are they ?



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Background

turbulent kinetic energy

$$k = \left(\frac{1}{2}\right) (\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) = \left(\frac{3}{2}\right) \overline{u'^2} \text{ if isotropic}$$

Favre (density-weighted) average

$$\tilde{u} = \frac{\overline{\rho u}}{\bar{\rho}} = \frac{\overline{(\bar{\rho} + \rho')(u + u')}}{\bar{\rho}} = \bar{\rho} \frac{\bar{u}}{\bar{\rho}} + \frac{\overline{\rho' u'}}{\bar{\rho}} \quad \text{so:}$$

$$\tilde{u} = \bar{u} + \frac{\overline{\rho' u'}}{\bar{\rho}}$$

replacing mean quantities in Navier Stokes Equations with their Favre averages removes all the density fluctuations - this removes one unknown (ρ') but it adds one new unknown: turbulent mass flux: $\overline{\rho' u'}$ which we determine using:

$$\overline{\rho' u'} = -D_T \frac{\partial \bar{\rho}}{\partial x} \quad \text{Prandtl's gradient diffusion assumption}$$



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Gradient diffusion assumption - relates Favre avg to time average

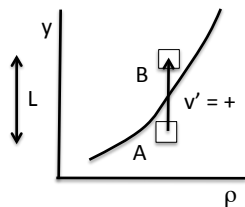
$$\tilde{u} = \bar{u} + \frac{\overline{\rho' u'}}{\bar{\rho}}$$

Favre average gets rid of one unknown (ρ') but introduces another one: $\overline{\rho' u'}$

$$\overline{\rho' u'} = -D_T \frac{\partial \bar{\rho}}{\partial x}$$

$$\overline{\rho' v'} = -D_T \frac{\partial \bar{\rho}}{\partial y}$$

Gradient
Diffusion
assumption



Suppose $\frac{\partial \bar{\rho}}{\partial y}$ and v' are positive

Small element will carry a low density from A To the higher density region at B. Therefore fluid at B will see a low density fluctuation, thus ρ' is negative at B

So: $\rho' = -L \frac{\partial \bar{\rho}}{\partial y}$ where L = integral scale

Thus $\overline{\rho' v'} = -L v' \frac{\partial \bar{\rho}}{\partial y}$ taking time average \rightarrow eqn above

We also proved that $D_T = v' L$



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Mixing: Turbulent viscosity = diffusivity is large

Since molecular viscosity $\mu / \rho = (\text{speed of sound}) (\text{mean free path})$

Prandtl suggested: $\mu_T / \rho = (u' L) \quad L = \text{integral scale}$

Dissipation rate of TKE $\epsilon = u'^3 / L \quad \text{see turbulence text by Tennekes}$

Since $u' = k^{1/2}$ then $\epsilon = k^{3/2} / L$ or $L = k^{3/2} / \epsilon$

Since we said above $\mu_T = \rho (u') (L)$, then: $\mu_T = c_\mu \bar{\rho} \frac{k^2}{\epsilon}$

How do we compute k and ϵ ? Prandtl suggested the k - equation

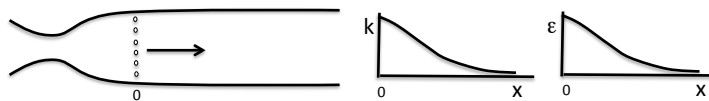


How to compute turbulence level k and dissipation rate ϵ ?

$$\bar{\rho} \tilde{u} \frac{\partial k}{\partial x} + \bar{\rho} \tilde{v} \frac{\partial k}{\partial y} = \frac{\partial}{\partial y} \left(\mu_T \frac{\partial k}{\partial y} \right) + \mu_T \left(\frac{\partial \tilde{u}}{\partial y} \right)^2 - \bar{\rho} \epsilon \quad \text{k-epsilon equations}$$

$$\bar{\rho} \tilde{u} \frac{\partial \epsilon}{\partial x} + \bar{\rho} \tilde{v} \frac{\partial \epsilon}{\partial y} = \frac{\partial}{\partial y} \left(\mu_T \frac{\partial \epsilon}{\partial y} \right) + C_\epsilon C_D \bar{\rho} k \left(\frac{\partial \tilde{u}}{\partial y} \right)^2 - \frac{C_\epsilon \bar{\rho} (\epsilon)^2}{C_D k}$$

convection = diffusion + creation - destruction



Example: Grid in a Wind tunnel $\bar{\rho}, \tilde{u}$ are constant, $\frac{\partial}{\partial y} = 0$ at $x > 0$ behind grid

Given: at $x = 0$ (grid) $k = k_0 = 10 \text{ m}^2/\text{s}^2$ and $\epsilon = \epsilon_0 = 1 \text{ (m/s)}^3/\text{m}$ then integrate:

$$\tilde{u} \frac{\partial k}{\partial x} = -\epsilon \quad \text{and} \quad \tilde{u} \frac{\partial \epsilon}{\partial x} = -\frac{C_\epsilon (\epsilon)^2}{C_D k} \quad \text{Solve on MATLAB}$$



Non – premixed turbulent flames

Mixture fraction (Z) = mass fraction of H-atoms

$$Z = (Y_H - Y_{H,2}) / (Y_{H,1} - Y_{H,2})$$

Y_H = mass fraction of H atoms contained in all molecules at a point

$Y_{H,1}$ = mass fraction of H atoms entering in stream 1

$Y_{H,2}$ = mass fraction of H atoms entering in stream 2 = 0 for our examples

Ex. Suppose a jet of methane CH₄ is surrounded by a large stream of pure O₂.
Stream 1 = methane, $Y_{H,1} = 4/16 = 0.25$, Stream 2 = O₂, so $Y_{H,2} = 0.0$

At some point P downstream suppose we have 2 moles H₂O and 1 mole CO₂.
At that point,

$$Y_H = \{ 4 \text{ g} / [44 \text{ g} + 2(18 \text{ g})] \} = 0.05$$

$$Z = (Y_H - Y_{H,2}) / (Y_{H,1} - Y_{H,2}) = (0.05 - 0) / [0.25 - 0] = 0.20$$



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Conservation equations for, Z, mass fractions of H₂ and O₂

Now consider a planar 2-D jet of H₂ surrounded by a stream of O₂

$$\bar{\rho} \tilde{u} \frac{d\tilde{Y}_{H_2}}{dx} + \bar{\rho} \tilde{v} \frac{d\tilde{Y}_{H_2}}{dy} = \bar{\rho} D_T \frac{d^2 \tilde{Y}_{H_2}}{dy^2} + \overline{\dot{\omega}_{H_2}}$$

$$\bar{\rho} \tilde{u} \frac{d\tilde{Y}_{O_2}}{dx} + \bar{\rho} \tilde{v} \frac{d\tilde{Y}_{O_2}}{dy} = \bar{\rho} D_T \frac{d^2 \tilde{Y}_{O_2}}{dy^2} + \overline{\dot{\omega}_{O_2}}$$

$$\bar{\rho} \tilde{u} \frac{d\tilde{Y}_{H_2O}}{dx} + \bar{\rho} \tilde{v} \frac{d\tilde{Y}_{H_2O}}{dy} = \bar{\rho} D_T \frac{d^2 \tilde{Y}_{H_2O}}{dy^2} + \overline{\dot{\omega}_{H_2O}}$$

The rate at which H₂O is formed is related to rate H₂ is consumed:

$$H_2 + \frac{1}{2} O_2 \rightarrow H_2O \quad \overline{\dot{\omega}_{H_2O}} = \left(-\frac{18}{2}\right) \overline{\dot{\omega}_{H_2}} \quad \overline{\dot{\omega}_{O_2}} = \left(\frac{16}{2}\right) \overline{\dot{\omega}_{H_2}}$$

Inserting these into the above and put in terms of Z to get:

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

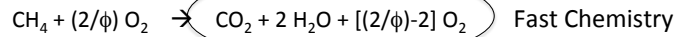
Mixture fraction
Conservation eqn
has no source term



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Flamelet idea: turbulent flame is filled with wrinkled, strained flamelets
State relation - relates mass fraction of O_2 at any point to mixture fraction Z

For our methane mixing into O_2 problem, for lean combustion at any equivalence ratio ϕ :



The gas mixture at any point that resulted from lean combustion must be the mixture in the oval. Assuming fast chemistry. How to relate ϕ to Z ?

For the mixture in the oval, $Z = 4 / [44 + 2(18) + (2/\phi - 2)32] / Y_{H,1}$, where $Y_{H,1} = 0.25$

Solve this for ϕ to get : $\phi = 4Z / (1-Z)$

Now what is Y_{O_2} for the mixture in the oval ? It is

$$Y_{O_2} = [(2/\phi)-2] 32 / \{44 + 36 + [(2/\phi)-2] 32\} = (4 - 4\phi) / (4 + \phi)$$

Insert into this the above formula for ϕ to get:

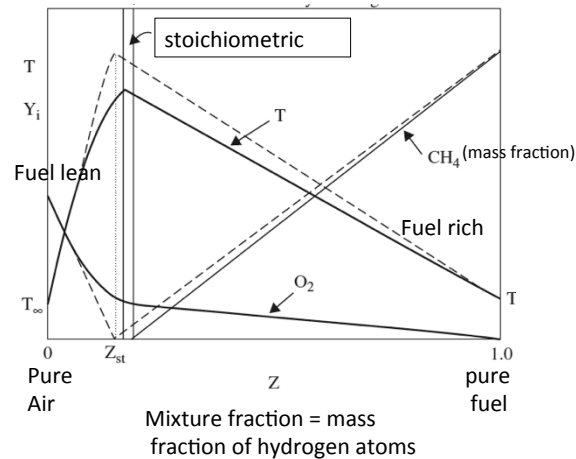
$$Y_{O_2} = (1 - 5Z)$$

(state relation for lean combustion, and Z only varies from 0 to 0.25)



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State relations for unstrained non-premixed flamelets



If you know the instantaneous mixture fraction (Z) at a point P , you use these state relations to look up instantaneous temperature and mass fractions at P



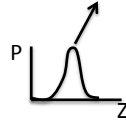
22

Probability density function - used to define a mean value

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

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

State relation =
Mass fraction of CO
Conditioned on Z



At each point in the flame, we solve conservation equations to get the mean mixture fraction and variance in mixture fraction $\overline{Z'^2}$

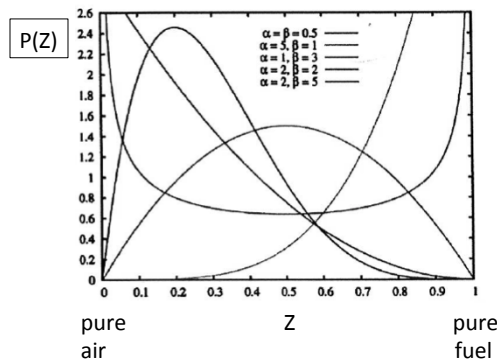
Idea: you only have to solve conservation equations for \bar{Z} and $\overline{Z'^2}$ and use above integral to get other mean values; you avoid solving more conservation equations for each variable



Assume PDF (Z) to be a Beta function for non-premixed flames

$$P(x; \alpha, \beta) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\int_0^1 u^{\alpha-1}(1-u)^{\beta-1} du}$$

here $x = Z =$ mixture fraction
 α and β are related to mean and variance of Z



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:

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

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



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

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

$$\bar{\rho} \tilde{u} \frac{d\bar{Y}_{CO}}{dx} + \bar{\rho} \tilde{v} \frac{d\bar{Y}_{CO}}{dy} = \bar{\rho} \alpha_T \frac{d^2 \bar{Y}_{CO}}{dy^2} + \bar{\dot{\omega}}_{CO} \leftarrow \text{kg/s/m}^3 \text{ CO produced} = ?$$

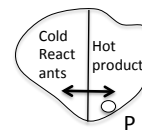
Turbulence-chemistry interaction – why do we need PDFs?

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:

$$\bar{\dot{\omega}}_{CO} = \bar{Y}_{fuel} \bar{Y}_{O_2} \exp(-E/R\bar{T})$$

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, O₂ and temperature

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

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



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

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



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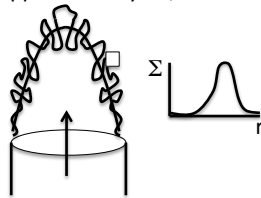
Premixed flame reaction rate depends on flame surface density

(FSD or Σ) = flame area per unit volume

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

A_f = average surface area of a premixed turbulent flame inside a small 1 mm³ interrogation box

P_f = average perimeter of flame boundary inside a 1 mm² 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

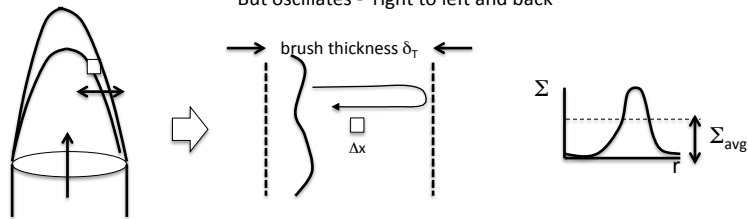


FSD is a Gaussian-like function in space



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: $\Delta x / \delta_\tau$

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

FSD should be independent of box size Δx

Average FSD = approx. $1 / \delta_\tau$ (= typically 0.2 mm⁻¹)



How to measure FSD ?

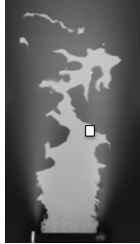


Image the flame boundary - using PLIF of OH or Mie scattering

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 mm³ interrogation box; vary the box location

Resulting value of FSD must be independent of interrogation box size

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

$$\Sigma = \text{approx. } [(\Delta x)^2 (\Delta x / \delta_T)] / (\Delta x)^3 \quad \text{so it should be independent of } (\Delta x)$$

$\delta_T = \text{brush thickness}$

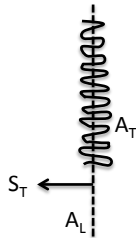


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Turbulence increases propagation speed - of a premixed flame

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



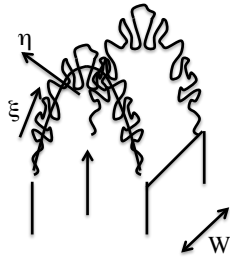
32

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

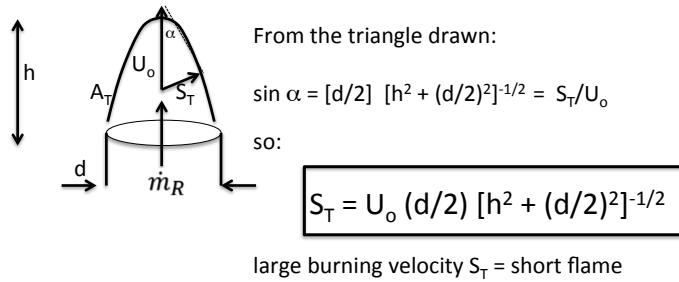


Second definition of turbulent burning velocity S_T

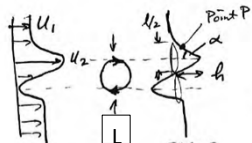
$S_{T,GC}$ = Global consumption speed

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

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



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 $(U_2 - S_L) \sin \alpha$, so equating these gives:

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

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

$$\alpha_T = c_2 u' L$$

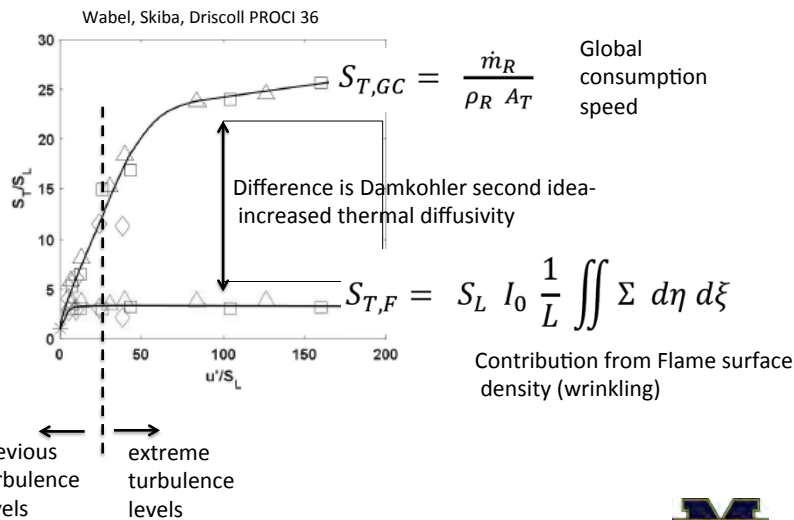
turbulent diffusivity = velocity fluctuation times integral scale L; ν = kinematic viscosity

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

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



Turbulent burning velocity at "extreme" turbulence levels



Turbulent burning velocity – what do we know ?

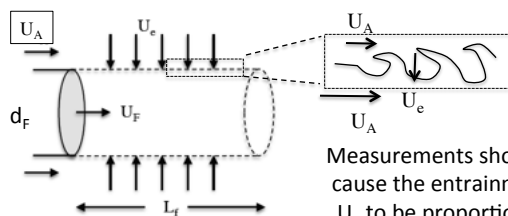
1. Six major canonical geometries for premixed turbulent flames
Bunsen, jet, low-swirl, V, spherical and swirl (Gas Turbine)
2. Burning velocity formula is different for each
3. Residence time (x/U) is important, bunsen flame tip becomes more wrinkled than flame base, spherical flame gets more wrinkled 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

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



40

Combine the above relations to eliminate U_e and solve for L_f to give :

$$\frac{L_f}{d_F} = \frac{c_2}{f_s} \left(\frac{\rho_F}{\rho_A} \right)^{1/2} \frac{U_F}{|c_1 U_F - U_A|}$$

Length of a jet flame
with co-axial air

If there is no co-flow (U_A is zero) the turbulent eddies at the edge of the cylinder are created by the jet velocity U_F so U_e is prop. to U_F and the above reduces to:

$$\frac{L_f}{d_F} = \frac{c_3}{f_s} \left(\frac{\rho_F}{\rho_A} \right)^{1/2}$$

Length of a jet flame
with NO co-axial air
 H_2-O_2 has large f_s = short

If there is strong co-flow air velocity, as in a gas turbine engine or rocket, then We neglect $c_1 U_F$ with respect to U_A so the above reduces to:

$$\frac{L_f}{d_F} = \frac{c_2}{f_s} \left(\frac{\rho_F}{\rho_A} \right)^{1/2} \frac{U_F}{|U_A|}$$

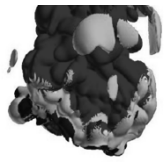
Length of a jet flame with
STRONG co-axial air
larger air velocity = shorter



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Flame Liftoff and Blowout

Base of a lifted, jet flame
that is initially non-premixed



A lifted initially non-premixed jet flame
has a partially-premixed flame base

DNS of Mizobuchi, Takeno
red= rich premix, blue = lean
premix green = non-premix
PROCI 30, 2005

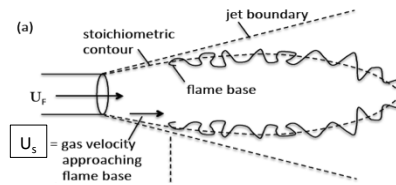
Cases of interest:

- Fuel jet with no coflow air (flame base is partially premixed)
- Fuel jet with cold coflow air (base is partially premixed)
- Fuel jet w very hot coflow air (base is not a flame, is auto ignition)
- Fuel jet in hot cross flow (base is not a flame, is auto ignition)
- Fuel jet w swirled air (base is partially premixed)
- Cavity stabilized flame (premixed in shear layer at top of cavity)



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Definitions



Consider a fuel jet issuing into air (initially non-premixed) with

U_f = jet exit velocity Z_s = stoichiometric mixture fraction = 0.055 for methane

U_s = axial velocity of gas along the stoichiometric contour; theory says:

U_s = **constant** - along the stoichiometric contour and this constant is $= U_f Z_s$

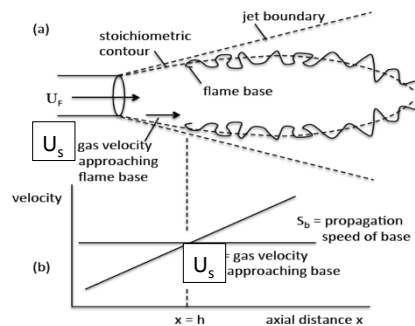
Why? See Kuo, conservation equations for mixture fraction (Z) and (u/U_f) are identical for a jet flame

Shear layer at fuel/air boundary is **premixed** upstream of lifted flame base

S_{base} = turbulent burning velocity – propagation speed of flame base against incoming reactants



Stability criterion (VanTiggelen, Comb Flame 10, p. 59)



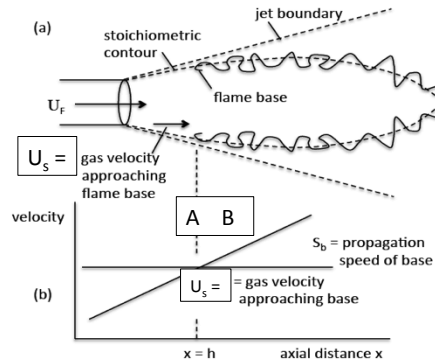
Two requirements
For flame to be stable:
 $U_s = S_{base}$
 $\partial S_{base}/\partial x > \partial U_s/\partial x$

Experiments show: The propagation speed (S_{base}) decreases in the negative-x direction since strain rate on the flame increases as you approach the fuel tube
In last slide we argue that U_s is constant in x-direction

notice that the slope $dS_{base}/dx > dU_s/dx$ in this plot



Stability



Flame normally is at location A where the two curves cross ($U_s = S_{\text{base}}$)

Suppose the flame base was perturbed to move downstream to location B
 Since $\partial S_{\text{base}} / \partial x > \partial U_s / \partial x$, it follows that $S_{\text{base}} > U_s$ at location B, this means
 That the flame will propagate upstream at speed ($S_{\text{base}} - U_s$) until it reaches A

This flame is stable – a perturbation causes it to return to its original position !



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Scaling Analysis – for Liftoff height, Blowout velocity jet flame

we said: $U_s = S_{\text{base}}$ and $U_s = U_F Z_s$

now we need a formula to estimate S_{base}

Define Karlovitz number = nondim strain rate = $(U_s / x) / (S_L / \alpha)$

Assume: $S_{\text{base}} = S_L [1 + Ka]^{-2}$ if Ka is large, S_{base} is small

S_L = laminar burning velocity, stoichiometric

Liftoff height $h = x$ and we said: $U_s = U_F Z_s$

Combine above, liftoff height is: $h = \{c_1 U_F / (S_L^2 / \alpha)\} F$

where function F is nearly constant

Larger jet velocity U_F – higher liftoff height



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Blowout velocity of a jet flame

There is no stoichiometric location downstream of $x = L_f =$ mixing length to stoich.

So when liftoff height (h) of flame base exceeds (L_f) – blowout occurs

$$h = L_f \quad L_f = c_2 d_F Z_s^{-1} \quad \text{from previous slide}$$

$$h = c_1 U_F / (S_{L,0}^2 / \alpha) \quad \text{from previous slide}$$

Combine these three equations and solve for U_F

Blowout fuel velocity:
$$U_F = c_3 d_F / (S_L^2 / \alpha) / F$$

RESULT: Liftoff and blowout formulas agree with measurements !
Don't make fuel injector diameter d_F too small



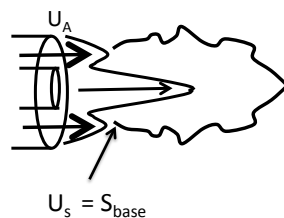
47

Co-flowing air is de-stabilizing

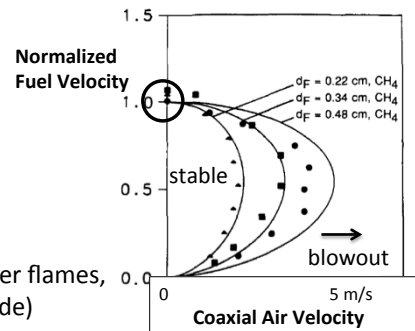
Co-flow air flows at velocity U_A , as shown below

Co-flow adds a velocity of U_A to U_s , at every point along the stoichiometric contour (red line)

Since $U_s = S_{base}$, the flame base must propagate against a larger velocity, so you must reduce the fuel velocity to avoid blowout



But co-flow air promotes shorter flames, faster mixing (see previous slide)



Feikema, Chen, Driscoll, Combust. Flame 80, 1990

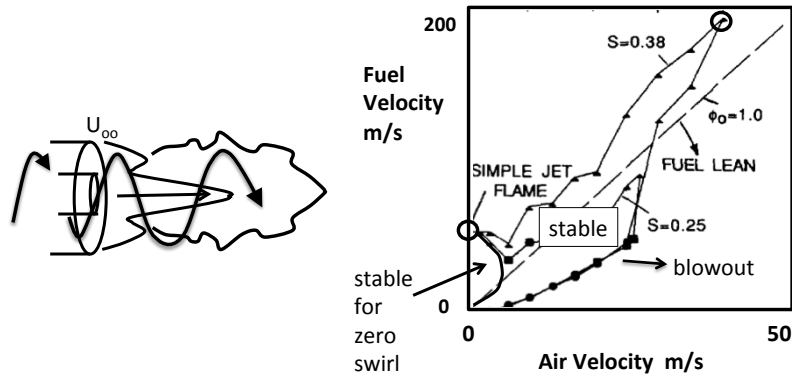


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Swirl is both STABILIZING and promotes faster mixing

so all gas turbine designs employ swirl
swirl creates internal recirculation = low gas velocities

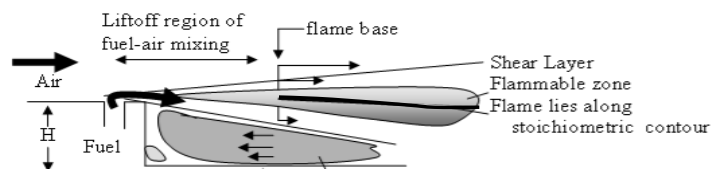
Much larger fuel Velocity achieved with swirl



Feikema, Chen, Driscoll, Combust. Flame 80, 1990



Scramjets use wall cavities to stabilize the flame



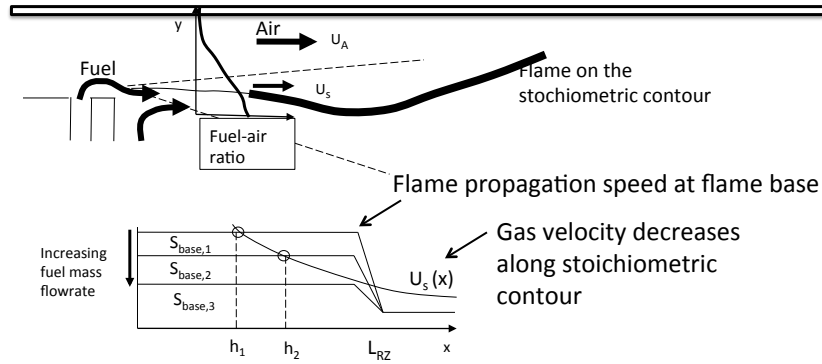
Air enters across upper side of shear layer

Fuel and hot products from recirculation zone enter across lower side of shear layer

Flame exists along stoichiometric contour



Blowout of cavity-stabilized flame – same ideas as before

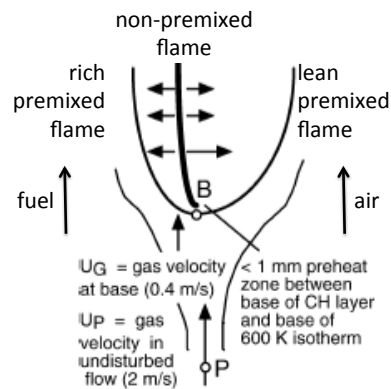


1. Liftoff height (h) where propagation speed (S_{base}) = gas velocity U_g
2. Temperature at base is elevated due to hot recirculation zone
3. Too much cold fuel into RZ lowers temperatures, flame speed
4. When liftoff height h exceeds L_{RZ} = "rich blowout"
5. Stable if $\partial S_{base} / \partial x > \partial U_s / \partial x$



Base of a lifted flame is a "triple flame"

How fast does a triple flame propagate ?



References - Flame blowout

Vanquickenborne L, van Tiggelen A. Combust Flame 1966;10, p. 59

Kalghatgi G. Blowout stability limits. Combust Sci Technol 1981; 26, p. 233.

Kalghatgi G. Liftoff heights of jet diffusion flames. Combust Sci Technol 41: p.17.

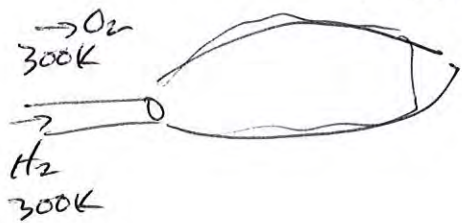
Brown C, Lyons K Studies on lifted jet flames in coflow. Flow Turb Comb 1999, p. 249.

Driscoll, J. F. Correlation and Analysis of Blowout Limits of Flames in High-Speed Airflows, J. Propulsion Power 21, 6,1035, 2005

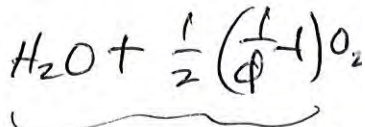
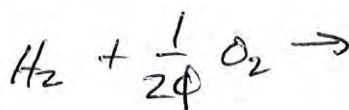
Mizobuchi, Takeno, PROCI 30, p. 611, 2005



state relation for gas temperature



P_0 lean location

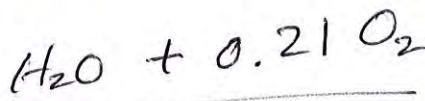


fictitious mixture that created mixture at P

$\text{O}_2 + P$ exists at P
actual gas mixture at P

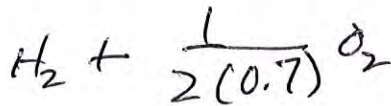
suppose $\phi = 0.7$

mixture at P is

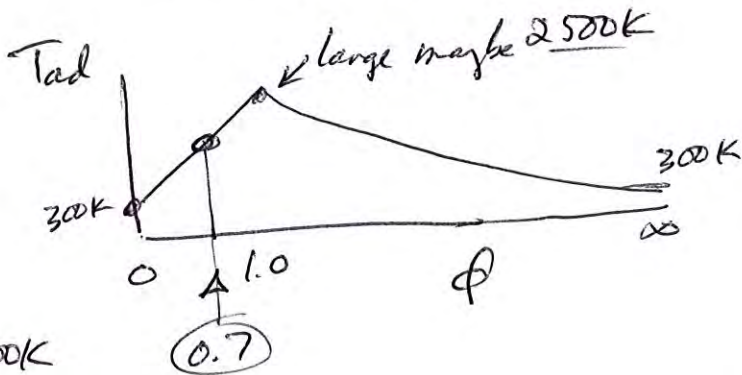


for this gas mixture the temperature must be the adiabatic flame temperature

associated with burning



so compute



\therefore pure H_2O must be at very high $T \approx 2500\text{K}$

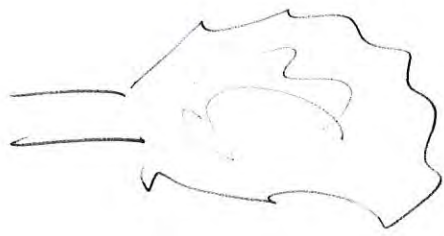
pure H_2 must be at 300K

cannot have pure H_2O at 300K !
cannot have pure H_2 at 2000K !

H_2O created at high T + mixed with $\text{O}_2 \rightarrow$ must cool due to dilution

! equal diffusivities

Turbulent Combustion ideas



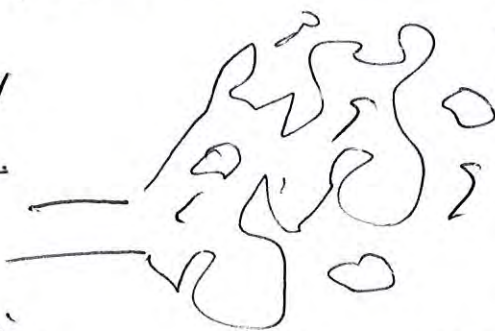
look at the fuzzy turbulent flame on handout - our gas turbine experiment - what is happening inside?

Damköhler proposed two ideas (1920's)

1. flamelet "model"

low levels of turbulence wrinkles

a "laminar-like" thin flamelet - called flamelets



continuous + pockets

flamelet - called flamelets

{ maybe continuous
maybe pockets
maybe segment / extinction

OR

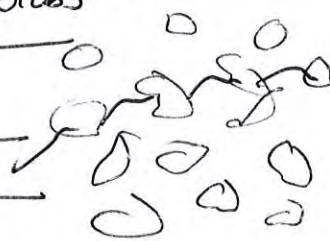
2. "perfectly stirred reactor" blobs

high levels of turbulence

creates blobs - each is

a perfectly stirred reactor

(computed on chemistry)



- must specify T_i, Y_{Fi}, Y_{O_i} etc +

residence time, mix time

SZF model (flamelets)

Chemkin C-Flow flamelets

⇒ [statistical avgs]

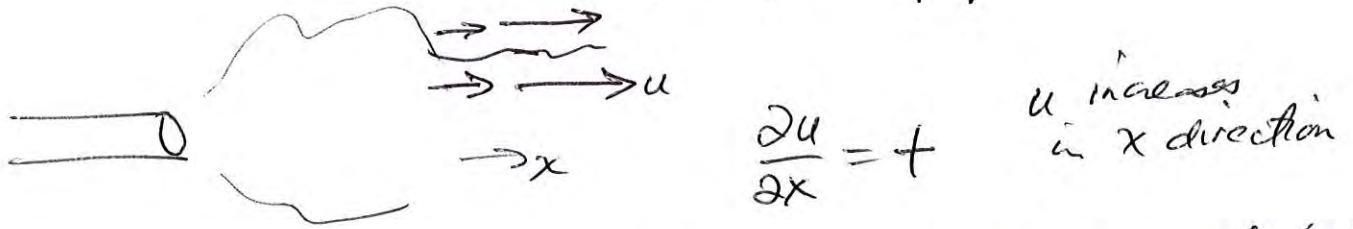
Pope's model (PSR blobs)

Chemkin PSR

⇒ [statistical avgs]

flamelet idea (Peters)

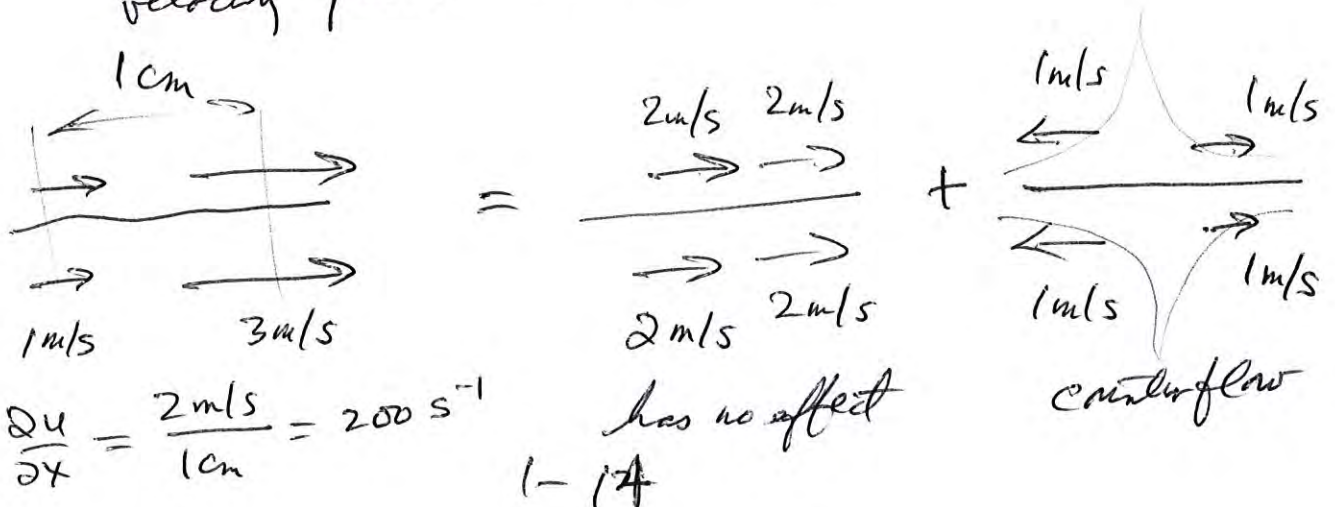
consider nonpremixed (or premixed) flamelet segment
in a velocity gradient



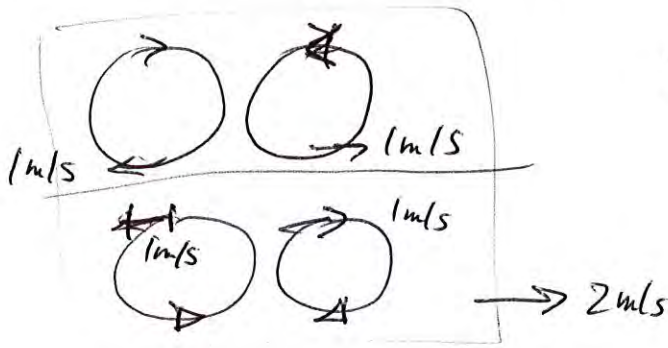
- a tangential velocity that is constant in space (+time)
does not alter a premixed or non premixed ^{laminar} flame

all our equations for PM or NPM flames are 1-D and
have no tangential velocity in the eqns
but if you add a constant tang. velocity, the
only terms are $\frac{\partial v}{\partial x}$ which is zero if $v = \text{const}$

- a tangential velocity that is not constant in space
 $\frac{\partial v}{\partial x} \neq 0$ exerts strain - any strain
velocity field can be decomposed



how does turbulent eddy exert this strain field

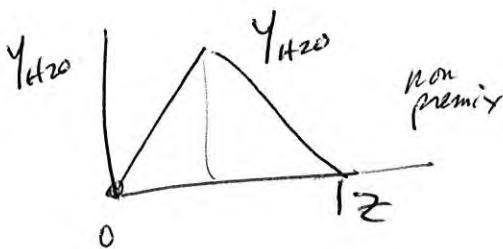


four eddies all move at 2 m/s to right

∴ we can model segment of wrinkled turb. flame (= flamelet) as counterflow flame but we need to know the rotational velocity i.e. velocity gradient = strain rate

chemkin does this! solves counterflow flamelet eqns

→ profiles of T, γ_i thru turbulent flamelet as fun of z are same as thru laminar C-F flame for the same velocity gradient $\frac{\partial u}{\partial x}$ ⇒ these are the "state" relations



still need to solve for $z = z(x, r)$ but can use state relation "mapping" when want Y_{H2O}, T , etc.

Flamelet analogy (Peters)

Turbulent non premixed flames are made up of thin and nearly-continuous reaction zones that have an internal structure that is similar to a strained laminar counterflow flame.

The rotation of velocity vectors due to turbulent eddies exerts a strain rate on the turbulent flamelets that can be approximated by the strain rate on a counterflow laminar flame

So we consider a simple counter flow non-premixed flame

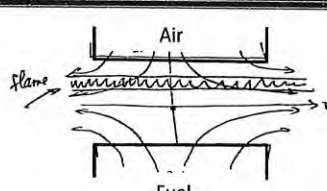
3 types of counterflow analysis

1.) constant density, fast chemistry (error free.)
 2.) full chemistry, variable density (CHEMKIN)
 3.) Flamelet eqn - neglect convection, assume $D_i = \text{const}$, full chemistry, incl. extinction

equal D_i
 too complex for turb. flame models
 variable D_i

Kup page 161

Counter flow non-premixed flame (Peters)



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

$\rho u \frac{dz}{dx} + \rho v \frac{dz}{dy} = \rho D \frac{d^2 z}{dy^2}$ so


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

so: $(-\epsilon y) \frac{dz}{dy} = D \frac{d^2 z}{dy^2}$

Assume:

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

b.c.: $y = \infty, Z = 0, y = -\infty, Z = 1$

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erf = error function = $(2/\sqrt{\pi}) \int_0^y \exp(-t^2) dt$
 erf = -1 at $y = -\infty$ and is 0 at $y = 0$ and is +1 at $y = +\infty$

derivative of erf (y) is: $(2/\sqrt{\pi}) \exp(-y^2)$

derivative of $(1/2 - 1/2 \operatorname{erf}(y/\sqrt{2D/\epsilon})) = -1/2 \cdot 2/\sqrt{\pi} \exp(-y^2/2)$

second deriv of $(1/2 - 1/2 \operatorname{erf}(y/\sqrt{2D/\epsilon})) = -1/2 \cdot 2/\sqrt{\pi} (y) \exp(-y^2/2)$

so this is soln to above ODE

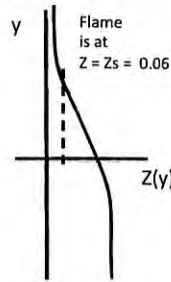
Solution to this equation is:

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

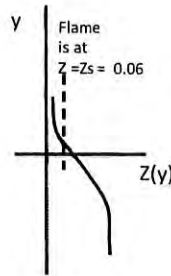
Scalar dissipation rate:

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

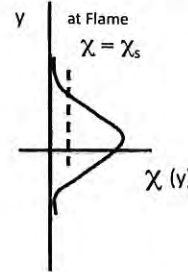
erf y



For low strain rate ϵ



For high strain rate ϵ
Larger gradient



$$\chi_s = \text{constant} \cdot \epsilon$$



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What is flame location ($y = y_f$) ? In solution for Z, set $Z = Z_s$ and solve for y

$$y_f = \sqrt{\frac{2D}{\epsilon}} \operatorname{erf}^{-1}(1 - 2Z_s) \quad \text{Flame location}$$

Flame location:

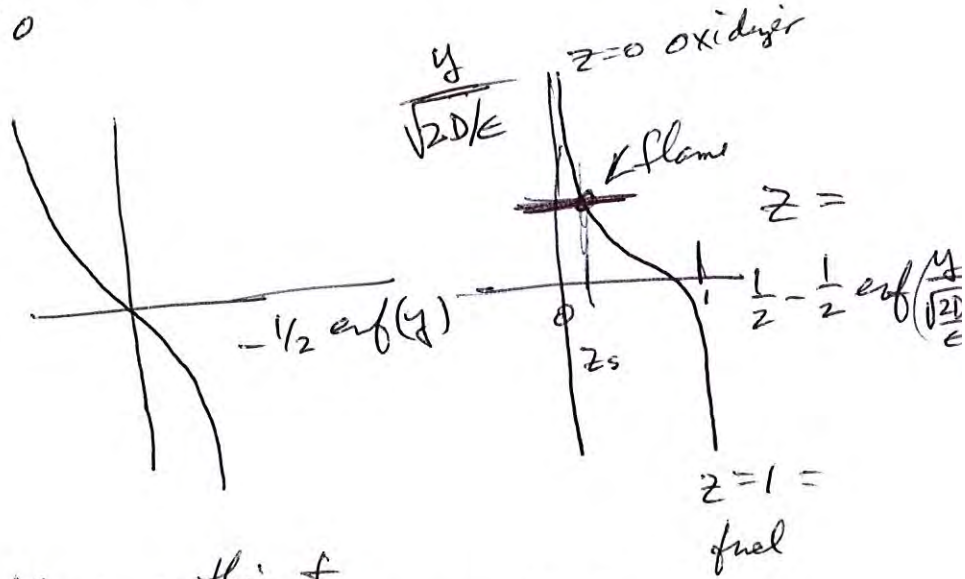
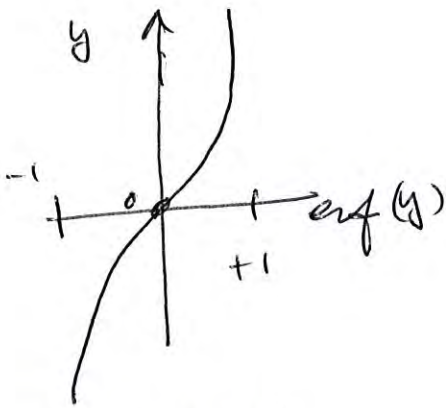
Increasing D $\rightarrow y_f$ increases

Increasing ϵ or $f_s \rightarrow y_f$ decreases



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$$\text{erf} = \frac{2}{\sqrt{\pi}} \int_0^y \exp(-t^2) dt$$



(simplified)
Counterflow flame

flame is within δ
is at $z = z_s$

$$= 0.111 \text{ H}_2\text{-O}_2$$

$$= 0.029 \text{ H}_2\text{-air}$$

$$= 0.067 \text{ Jet A-air}$$

$$C_{10}H_{20}$$

define $\chi(y)$, χ_s

$$u = \epsilon x$$

$$\epsilon = \text{velocity strain rate} = \frac{\partial u}{\partial x} = -\frac{\partial v}{\partial y}$$

Strength of a strained non-premixed counterflow flame

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

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

$$J_F = -\rho_F D \frac{\partial Y_F}{\partial y} \quad \text{Ficke's Law}$$

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

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

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

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

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



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

Define scalar dissipation rate for this counter flow geometry

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

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

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

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

So the scalar gradient is related to velocity gradient



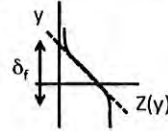
24

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

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

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



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

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

Flame gets thinner as you apply more strain

Example: if $D = 1.0 \text{ cm}^2/\text{s}$ = gas diffusivity near flame

if dissipation rate $\chi_s = 100 \text{ s}^{-1}$

Then flame thickness: $\delta_f = 1.4 \text{ mm}$



AN INTRODUCTION TO COMBUSTION

Concepts and Applications

SECOND EDITION

This describes how CHEMKIN computes a counterflow non premixed flame

Stephen R. Turns

Counterflow Flames

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COUNTERFLOW FLAMES¹

In the past few decades, many theoretical and experimental studies have been conducted on flames fed by opposing jets of fuel and oxidizer (Fig. 9.15). Such flames are of fundamental research interest because they approximate a one-dimensional character and because residence times within the flame zone can be easily varied. In the previous section, we saw the complexities associated with the 2-D (axisymmetric) jet flame; in contrast, the one-dimensionality of the counterflow flame makes both experiments and calculations much more practicable. For example, in experiments, temperature and species conservation measurements need only be made along a single line; while in theoretical studies, only modest run times are needed for computations using extremely complex chemical kinetics (cf. Table 5.3). The counterflow flame provides fundamental understanding of the detailed structure of diffusion flames and their extinction characteristics. Furthermore, the laminar counterflow flame has been proposed as a fundamental element in the complex structure of turbulent non-premixed flames [27] (Chapter 13). A rather large counterflow flame literature has developed (e.g., Refs. [28–31]), and continues to expand.

Before we present a mathematical description, it is important to understand the basic features of the counterflow flame. A typical experimental arrangement is illustrated in Fig. 9.15. Here we see opposing jets of fuel and oxidizer, which create a stagnation plane ($v_x = 0$) whose location depends on the relative magnitudes of the oxidizer and fuel jet initial momentum fluxes. For equal momentum fluxes ($\dot{m}_F v_F = \dot{m}_{O_x} v_{O_x}$), the stagnation plane lies at the midpoint between the nozzle exit planes; however, if the momentum flux of one

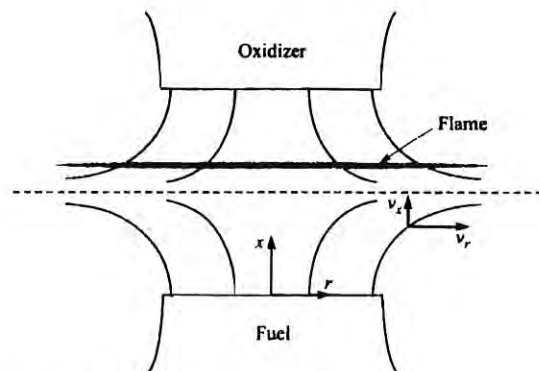


Figure 9.15 Counterflow diffusion flame lies above stagnation plane (dashed line) created by opposing streams of fuel and oxidizer.

5
1-21

stream is increased over the other, the stagnation plane moves closer to the low-momentum-flux stream outlet. Given appropriate conditions, a diffusion flame can be established between the two nozzles, the location of which is where the mixture fraction is nominally stoichiometric. For most hydrocarbon fuels burning in air, stoichiometric conditions require considerably more air than fuel ($f_{\text{stoic}} \approx 0.06$). In this case, then, the fuel must diffuse across the stagnation plane to the flame location, as shown in Fig. 9.15. Conversely, if a reactant pair in which more fuel than oxidizer is required for stoichiometric conditions ($f_{\text{stoic}} > 0.5$), the flame would lie on the fuel side of the stagnation plane. An important characteristic of the opposed flow is that the flame established between the nozzles is essentially flat (a disk for round nozzles) and one-dimensional, having dependencies only in the x -direction.

Mathematical Description

Two different approaches to modeling counterflow flames can be found in the literature. The first approach couples a stagnation-point potential flow from a point source at infinity with a boundary-layer type analysis (see, e.g., Ref. [31]). In this analysis, the finite separation between the nozzles cannot be taken into account. A second approach [32, 33] was developed that explicitly accounts for the flows exiting from the nozzles rather than being generated by a far-removed point source. The initial formulation of this model was developed for premixed flames [32] and, subsequently, was extended to nonpremixed flames [33]. This second approach is summarized briefly below. For additional details, the reader is referred to the original references [32, 33]. After presenting the model, we will examine the detailed structure of a CH_4 -air diffusion generated by a numerical solution.

The overall objective of the analysis is to transform the set of axisymmetric, governing, partial differential equations into a coupled system of ordinary differential equations, cast as a boundary-value problem. The continuity and conservation of momentum equations used as the starting point for the analysis are the axisymmetric forms given in Chapter 7: Eqn. 7.7 for mass conservation and Eqns. 7.43 and 7.44 for axial and radial momentum, respectively. To effect the desired transformation, the following stream function is employed:

$$\Psi \equiv r^2 F(x), \quad (9.75)$$

where

$$\frac{\partial \Psi}{\partial r} = r \rho v_x = 2rF \quad (9.76a)$$

and

$$-\frac{\partial \Psi}{\partial x} = r \rho v_r = -r^2 \frac{dF}{dx}. \quad (9.76b)$$

From the above, it is a simple matter to show that the stream function (Eqn. 9.75) satisfies continuity (Eqn. 7.7). To reduce the order of the radial momentum equation, discussed below, a new variable $G(\equiv dF/dx)$ is defined. This defining equation is the first ordinary differential equation in our set:

$$\frac{dF}{dx} = G. \quad (9.77)$$

Equations 9.76a, 9.76b, and 9.77 are now substituted into the momentum conservation relations, Eqns. 7.43 and 7.44, but buoyancy is ignored. The equations resulting from this substitution are of the following form:

$$\frac{\partial P}{\partial x} = f_1(x) \quad (9.78a)$$

$$\frac{1}{r} \frac{\partial P}{\partial r} = f_2(x). \quad (9.78b)$$

This result is used to generate an eigenvalue equation for the radial pressure gradient. From mathematical operations alone, we can relate the left-hand-sides of Eqns. 9.78a and 9.78b:

$$\frac{\partial}{\partial x} \left(\frac{1}{r} \frac{\partial P}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial x} \left(\frac{\partial P}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\partial P}{\partial x} \right).$$

Furthermore, since both $\partial P/\partial x$ and $(1/r)(\partial P/\partial r)$ are functions of x only, it follows that

$$\frac{\partial}{\partial x} \left(\frac{1}{r} \frac{\partial P}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\partial P}{\partial x} \right) = 0 \quad (9.79)$$

and

$$\frac{1}{r} \frac{\partial P}{\partial r} = \text{constant} \equiv H. \quad (9.80)$$

The radial-pressure-gradient eigenvalue, H , thus enters into the set of ordinary differential equations as

$$\frac{dH}{dx} = 0. \quad (9.81)$$

Since the pressure is uniform throughout the flowfield (low Mach-number approximation), we have no further use for the axial momentum equation (Eqn. 9.78a); the radial momentum equation, however, must be retained. Substituting Eqn. 9.80 into Eqn. 9.78b and fleshing out the right-hand-side results in the following:

$$\frac{d}{dx} \left[\mu \frac{d}{dx} \left(\frac{G}{\rho} \right) \right] - 2 \frac{d}{dx} \left(\frac{FG}{\rho} \right) + \frac{3}{\rho} G^2 + H = 0. \quad (9.82)$$

1-23

The corresponding energy and species conservation equations are, respectively,

$$2Fc_p \frac{dT}{dx} - \frac{d}{dx} \left(k \frac{dT}{dx} \right) + \sum_{i=1}^N \rho Y_i v_{i,diff} c_{p,i} \frac{dT}{dx} - \sum_{i=1}^N h_i \dot{\omega}_i M W_i = 0 \quad (9.83)$$

and

$$2F \frac{dY_i}{dx} + \frac{d}{dx} (\rho Y_i v_{i,diff}) - \dot{\omega}_i M W_i = 0 \quad i = 1, 2, \dots, N. \quad (9.84)$$

CHEMKIN counterflow
non premixed flame
-
assume:
d/dr = 0 except that
dp/dr is not zero
do not assume $u = \epsilon x$
do not say density = const
-
get vr from F equation
(from continuity)
-
get vx from G equation
(from axial mom eqn)
-
get p from H eqn
(from radial mom eqn)
-
get Yi from Yi eqn 9.84
-
get T from energy eqn 9.83
-
get p from eqn state

In summary, the counterflow diffusion flame model consists of the set of five ordinary differential equations (Eqns. 9.77, 9.81, 9.82, 9.83, and 9.84) for the four functions $F(x)$, $G(x)$, $T(x)$, and $Y_i(x)$ and the eigenvalue, H . In addition to these basic equations, the following ancillary relations or data are required:

- Ideal-gas equation of state (Eqn. 2.2).
- Constitutive relations for diffusion velocities (Eqns. 7.23 and 7.25 or Eqn. 7.31).
- Temperature-dependent species properties: $h_i(T)$, $c_{p,i}(T)$, $k_i(T)$, and $D_{ij}(T)$.
- Mixture property relations to calculate MW_{mix} , k , D_{ij} , and D_i^T from individual species properties and mole (or mass) fractions (e.g., for the D_{ij} s, Eqn. 7.26).
- A detailed chemical kinetic mechanism to obtain the $\dot{\omega}_i$ s (e.g., Table 5.3).
- Interconversion relations for χ_i s, Y_i s, and $[X_i]$ s (Eqns. 6A.1–6A.10).

Boundary conditions are applied at the two nozzle exits (Fig. 9.15), defined as $x \equiv 0$ at the fuel-nozzle exit and $x \equiv L$ at the oxidizer-nozzle exit, to complete the formulation of the boundary-value problem. The necessary conditions are the exit velocities and their gradients, exit temperatures, and exit species mass fractions (or mass flux fractions), which we specify as follows:

$$\begin{array}{ll} \text{At } x = 0: & \text{At } x = L: \\ F = \rho_F v_{e,F} / 2, & F = \rho_{Ox} v_{e,Ox} / 2, \\ G = 0, & G = 0, \\ T = T_F, & T = T_{Ox}, \\ \rho v_x Y_i + \rho Y_i v_{i,diff} = (\rho v_x Y_i)_F; & \rho v_x Y_i + \rho Y_i v_{i,diff} = (\rho v_x Y_i)_{Ox}. \end{array} \quad (9.85)$$

Structure of CH₄–Air Flame

We now employ the counterflow flame model described above to analyze the structure of a CH₄–air diffusion flame. The OPPDIF software described in Ref. [33], together with the CHEMKIN library codes [34], were used with chemical kinetics taken from Miller and Bowman [35]. Figure 9.16 shows computed

1-24

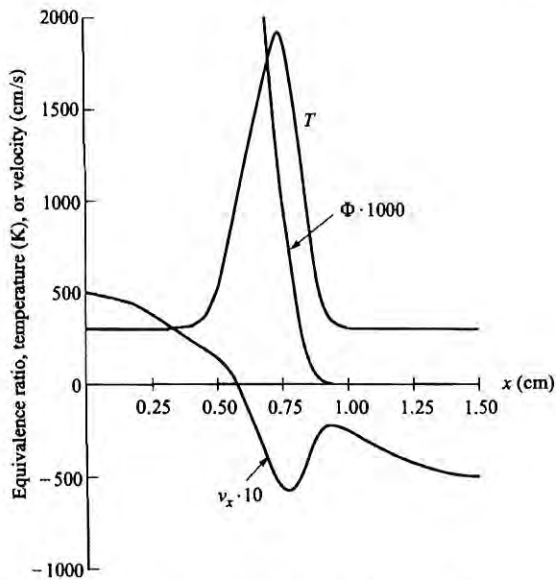


Figure 9.16 Equivalence ratio, temperature, and velocity profiles through CH_4 -air counterflow diffusion flame. The CH_4 and air streams both exit at 50 cm/s; $L = 1.5$ cm.

temperature and velocity profiles between the fuel (left) and air (right) nozzles, while Fig. 9.17 presents corresponding major species mole-fraction profiles. Also shown in Fig. 9.16 is the local equivalence ratio computed from carbon and nitrogen balances.

Focusing on the velocity profile, we see in Fig. 9.16 that the stagnation point ($v_x = 0$) lies to the left of the center plane between the two nozzle flows, as expected, since the higher density of air causes the momentum flux of the air stream to be greater than that of the fuel stream for equal outlet velocities (50 cm/s). The velocity profile exhibits interesting behavior in the heat-release region of the flame, where a minimum value ($v_x = -57.6$ cm/s) occurs slightly to the air side of the peak temperature. We note that this is the maximum absolute value of the velocity, as velocities directed to the left are negative. Simplistically, this result is understood as a consequence of continuity, with the gas speed increasing in response to the density decreasing. Frequently, a velocity gradient, dv_x/dx , is used to characterize the strain rate in counterflow flames; for the twin-nozzle geometry, the relatively long region of essentially constant slope before the velocity minimum is used as the characteristic gradient. For the particular case illustrated in Fig. 9.16, the value of the velocity gradient is approximately 360 s^{-1} .

As essential feature of nonpremixed flame is a continuous variation of the mixture fraction, f , or, alternatively, the equivalence ratio, Φ , from pure fuel at

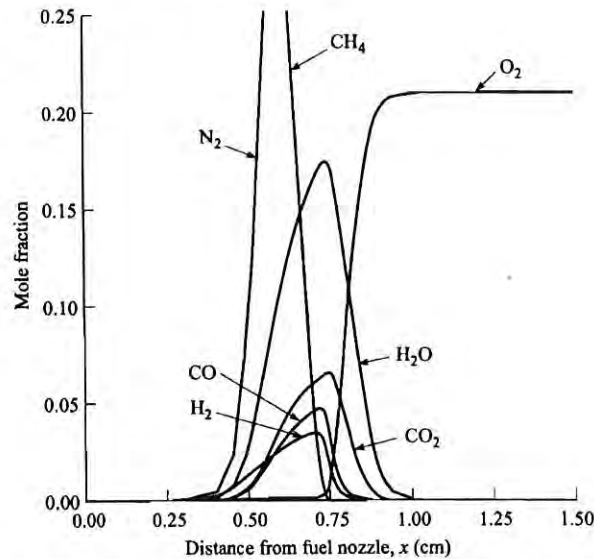


Figure 9.17 Major species mole-fraction profiles through CH_4 -air counterflow flame. Same conditions as Fig. 9.16.

the left nozzle ($f = 1$, $\Phi \rightarrow \infty$), to pure air at the right nozzle ($f = 0$, $\Phi = 0$). Figure 9.16 shows this variation of equivalence ratio over the range from 2 to zero. A close inspection of Fig. 9.16 reveals that the location of the maximum temperature occurs at a slightly rich stoichiometry ($\Phi = 1.148$), with temperatures about 40 K lower at $\Phi = 1$. From thermodynamic considerations alone, one expects peak temperatures to occur at slightly rich conditions (see Chapter 2). For our CH_4 -air system, the peak adiabatic flame temperature occurs at $\Phi = 1.035$. This value of Φ is considerably less rich than for the diffusion flame ($\Phi = 1.148$), where convection, diffusion, and chemical kinetics all combine to determine the peak-temperature equivalence ratio.

Turning now to the species profiles (Fig. 9.17), we focus first on the reactants. Here we see that both CH_4 and O_2 mole fractions fall to near-zero values at an axial location of approximately 0.75 cm; this corresponds closely with the occurrence of the peak temperature, as can be seen from Fig. 9.16. We also note some overlap, or simultaneous presence of CH_4 and O_2 , however small, in the region immediately preceding the maximum temperature. For the particular conditions of this simulation, the combustion kinetics are not sufficiently fast to obtain a true approximation to a flamesheet; thus, a distributed reaction zone results. Another interesting reactants-related feature of Fig. 9.17 is the presence of N_2 deep on the fuel side. Since all N_2 in the flame system has its origins with the air, the N_2 must diffuse across the stagnation plane to yield the relatively high concentrations we observe on the fuel side of the flame. Of

course, the presence of fuel to the right of the stagnation plane ($x = 0.58$ cm) is a result of diffusion in the direction opposite to the N_2 .

From Fig. 9.17, we see a progression of species mole-fraction maxima from left to right. This is illustrated more clearly by the data presented in Table 9.7, where we see that the H_2 peak occurs at the richest condition of all species shown, followed by the peaks of CO , H_2O , and CO_2 . All of these maxima occur at rich equivalence ratios, as might be expected for all but the CO_2 . Some effects of chemical kinetics can be illuminated by comparing the predicted mole fractions for the major species in the flame with equilibrium values based on identical temperatures and stoichiometry. Two such comparisons are shown in Table 9.8: the first, at the location of the maximum temperature, and the second, at the location of stoichiometric conditions. In both cases, we see substantially less CO_2 and H_2O in the flame compared with the equilibrium conditions. With lower levels of fully oxidized products (CO_2 and H_2O) in the flame, one expects incomplete products of combustion to appear in greater abundance. At the $\Phi = 1.0$ case, in particular, CO , H_2 , and O_2 levels are approximately 15–20 times higher in the flame.

Table 9.7 Location of peak species mole fractions and temperature in simulated CH_4 -air counterflow diffusion flame

Species	Maximum Mole Fraction	Location of Maximum, x (cm)	Φ	T (K)
H_2	0.0345	0.7074	1.736	1786.5
CO	0.0467	0.7230	1.411	1862.6
H_2O	0.1741	0.7455	1.165	1926.8
CO_2	0.0652	0.7522	1.085	1913.8

Table 9.8 Comparison of flame composition with that for adiabatic equilibrium at locations of maximum temperature and stoichiometric mixture fraction ($\Phi = 1$)

Condition	O_2	CO	H_2	CO_2	H_2O	N_2
			$T = T_{max} (1925.8 \text{ K}), \Phi = 1.148$			
Flame	0.0062	0.0394	0.0212	0.0650	0.174	0.686
Adiabatic equilibrium	$2.15 \cdot 10^{-6}$	0.0333	0.0207	0.0714	0.189	0.686
			$\Phi = 1.000, T = 1887.5 \text{ K}$			
Flame	0.0148	0.0280	0.0132	0.0648	0.170	0.697
Adiabatic equilibrium	0.0009	0.0015	0.0007	0.0934	0.189	0.714

CHEMKIN counterflow non premixed hydrogen-air flame

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Figure 2-13 Flame Speed—Axial Velocity vs. Distance

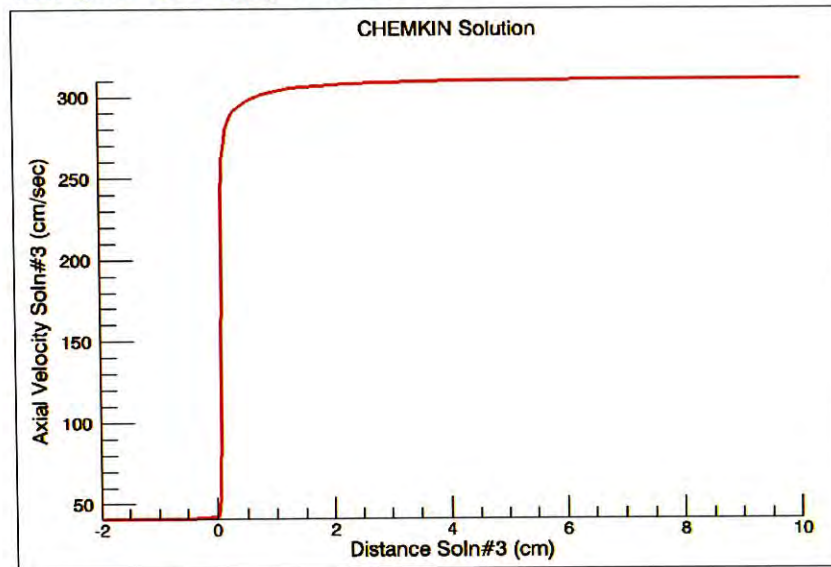
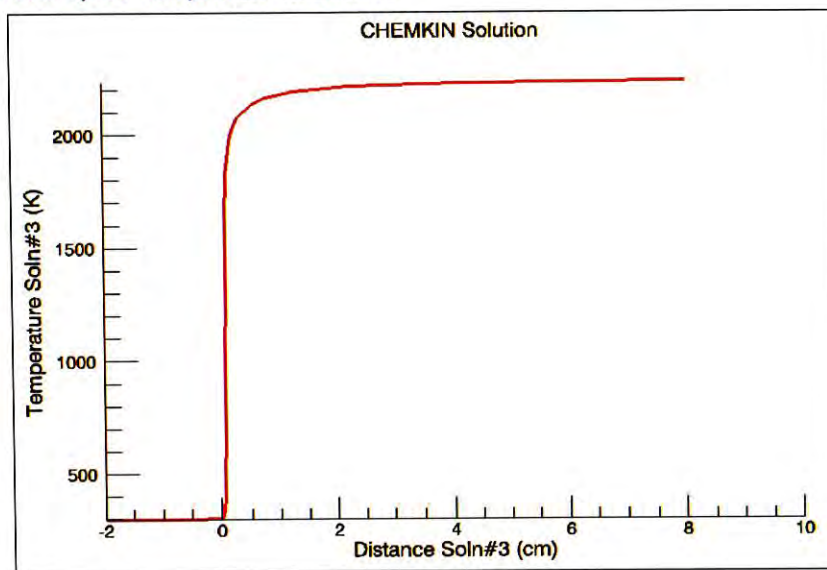


Figure 2-14 Flame Speed—Temperature vs. Distance



2.2.5 Hydrogen/Air Flame

2.2.5.1 Project Description

This user tutorial presents a simulation of opposed flow **diffusion flame** of hydrogen and air at low pressure. This project uses the chemistry set for hydrogen combustion described in [Section 2.6.1](#). The opposed-flow geometry makes an attractive experimental configuration, because the flames are flat, allowing for detailed study of the flame chemistry and structure. The two or three-dimensional flow is reduced

mathematically to one dimension. This problem uses cylindrical coordinates where one stream contains fuel and the other oxidizer. It also demonstrates the use of sensitivity analysis for reaction rates and species heats of formation. The latter analysis is useful for evaluating the effects of thermochemical parameters that may have been estimated, or have high uncertainties.

2.2.5.2 Project Setup

The project file is called *opposed-flow_flame_h2_air.ckprj*. The data files used for this sample are located in the *samples\opposed-flow_flame_h2_air* directory. This reactor diagram contains two gas inlets and one Opposed-flow Reactor.

On the Reactor Physical Property tab of the C1_R1 Opposed-flow Flame panel, the problem type of Solve Gas Energy Equation is selected. Here, the use of Mixture-averaged Transport properties is also selected, as is the choice of a plateau-shaped, rather than a linear, profile for the starting guess used in the simulation. An optional value for the maximum temperature to be used in the initial profile is provided to help convergence.

On the Initial Grid Property tab of the C1_R1 Opposed-flow Flame panel, the use of cylindrical geometry is selected for this problem, and the axial length of the simulation (2 cm) is input. In this reactor model, the fuel always enters the system at the origin, and the oxidizer inlet is located at the Ending Axial Position. The opposed-flow reactor model uses adaptive gridding, and in this case, the spacing of the 14 initial grid points have been specified by use of a profile file, *opposed-flow_flame_h2_air.ckprf*. There are 4 optional parameters on this panel that provide input for the adaptive gridding, two of which have values that we have input to override the defaults. The simulation also needs a starting estimate of the solution from which to begin its iteration, and the Estimated Center Position and Estimated (reaction) Zone Width help specify that. The gas composition giving the expected combustion products that are input on the Product Fraction sub-tab of the Species-specific Data tab on the C1_R1 Opposed-flow Flame panel are also part of the initial guess.

The gas inlet panels are named to reflect their function. The inlet gas velocities (100 cm sec^{-1}) are input on the Species-specific Data tabs of the Fuel and Oxidizer panels, along with inlet gas temperatures (300 K). The inlet gas compositions, pure hydrogen and pure air, are input on the Reactant Fraction sub-tab of the Species-specific Data tab of the Fuel and Oxidizer panels, respectively.

On the Solver panel, there are a number of inputs on the Basic and Advanced tabs to override the default values and assist convergence. On the Output Control tab of the Output Control panel, boxes are checked to request that sensitivity calculations be done for all variables with respect to both reaction-rate A factors and species heats of formation. On the Species Sensitivity tab, three species are listed as being Output Species. The A-factor Sensitivity and Heat of Formation check boxes for these species do not need to be checked here, because they are already covered by the request for All A-factor sensitivities on the Output Control tab, but this redundancy does no harm. There are no inputs on the Cluster Properties or Continuations panels for this project.

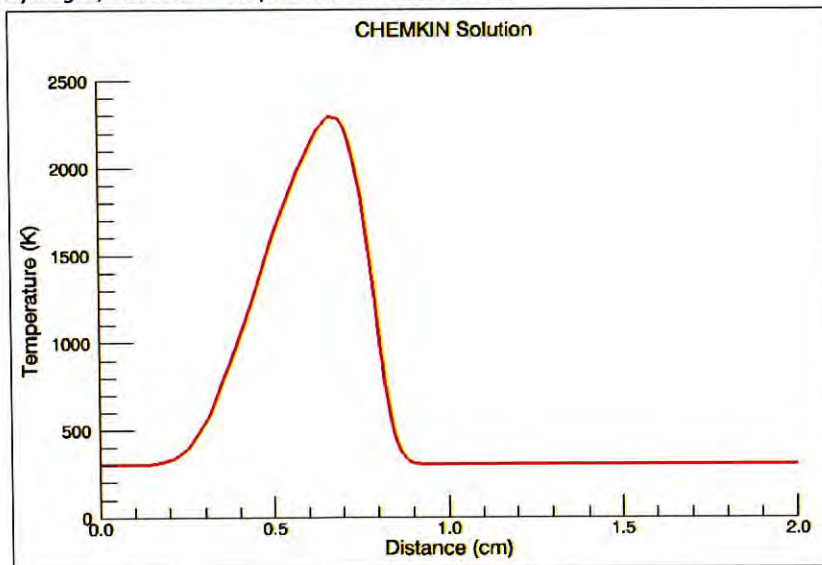
2.2.5.3

Project Results

Figure 2-15 shows the gas temperature from the simulation as a function of axial distance. The flame is located on the fuel side of the stagnation plane, which is a result of using hydrogen as the fuel. Most fuels require more air than fuel by mass, so the diffusion flame usually sits on the oxidizer side of the stagnation plane. In a stoichiometric mixture, the fuel usually diffuses through the stagnation plane to establish the flame. For H_2 however, more fuel is required than air. The mole fractions in *Figure 2-16* for the major species show that the flame sits on the fuel side of the stagnation plane in this case. An inspection of the text file shows that the simulation now has 45 grid points, a significant increase from the initial 14 grid points.

Figure 2-15

Hydrogen/Air Flame—Temperature vs. Axial Distance



"Flamelet Equation" to get realistic "State Relations" for finite rate chemistry

$$\rho \frac{\chi}{Z} \frac{d^2 Y_i}{dz^2} = -\dot{w}_i$$

steady flamelet equation
 - no convection terms
 - full chemistry including extinction

derived in Peters "Turb. Comb." p. 208
 see FLUENT section 15.3.6

idea: remove (x, y) from the counterflow conservation eqns, replace with z = mixture fraction using chain rule. Flamelet eqn is simpler than chemkin eqns for F, G, H, Y, T - has full chemistry

$$\frac{\partial^2 Y_{H_2}}{\partial x^2} = \frac{\partial^2 Y_{H_2}}{\partial z^2} \left(\frac{\partial z}{\partial x} \right)^2$$

$$\frac{\partial^2 Y_{H_2}}{\partial y^2} = \frac{\partial^2 Y_{H_2}}{\partial z^2} \left(\frac{\partial z}{\partial y} \right)^2$$

add

$$\frac{\partial^2 Y_{H_2}}{\partial x^2} + \frac{\partial^2 Y_{H_2}}{\partial y^2} = \frac{\partial^2 Y_{H_2}}{\partial z^2} \left(\left(\frac{\partial z}{\partial x} \right)^2 + \left(\frac{\partial z}{\partial y} \right)^2 \right)$$

these are in C-F conservation eqns, based on physical coords (x, y)

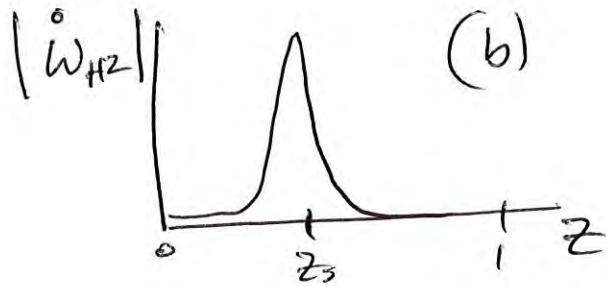
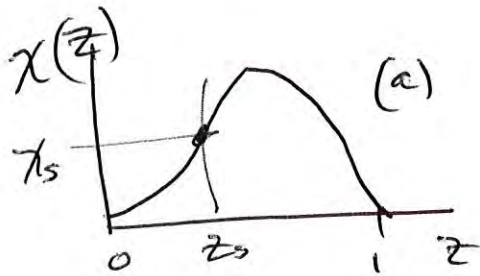
↑ this is term on LHS above

X / 2D

↑ this is where X comes from

no (x, y) spatial coords
 steady
 need $\rho(z), \chi(z)$ and $\dot{w}_i(z)$ to solve

to solve the flamelet equation we need to represent
 $\chi(z) = ?$ $\dot{w}_i(z) = ?$



in our C-F flame solution
 we had an erf solution
 showing that $\chi = 0$ at
 $z = 0$ (pure air side) and
 at $z = 1$ (pure fuel side)
 $\chi_s =$ diss. rate at $z = z_s$
 $z_s = 0.111$
 for $H_2 - O_2$

$\dot{w}_i = 0$ at $z = 0$ or 1
 $\dot{w}_i = \text{max}$ near $z = z_s$

approach = assume a functional form of $\chi(z)$

$$(i) \quad \chi_z(z) = \chi_s \frac{\exp\{-2 [\text{erfc}^{-1}(2z)]^2\}}{\exp\{-2 [\text{erfc}^{-1}(2z_s)]^2\}}$$

↑
given

this function has the shape plotted in (a) above

(ii) set $\dot{w}_{H_2} =$ Arrhenius relation - many terms $w(Y_i, T)$
 use state relations to relate Y_i, T to z

Now we can solve flamelet eqn if we are given χ_s

Derivation of the Flamelet Equation,
Eqn. 3-134 on next page
Peters, N. Turbulent Combustion, p. 208

species conservation eqn	$\rho \frac{\partial \psi_i}{\partial t} + \rho \mathbf{v} \cdot \nabla \psi_i = \nabla \cdot (\rho D_i \nabla \psi_i) + \omega_i.$	(3.123)
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The short scale in the two-scale asymptotic analysis is defined by

$$\zeta = \varepsilon^{-1}(Z(\mathbf{x}, t) - Z_{st}). \quad (3.124)$$

This short-range coordinate covers the vicinity normal to the instantaneous flame surface, while the flow and the mixing field further away is described by the long-range spatial coordinates \mathbf{x} and the long time t . In the new coordinate system ξ replaces \mathbf{x} and the short time scale

$$\tau = \varepsilon^{-2}t \quad (3.125)$$

is introduced to describe rapid temporal changes of the flamelet structure in the vicinity of the surface of stoichiometric mixture.

The reactive scalars are expanded into a leading order and a first-order term as

$$\psi_i = \psi_i^0 + \varepsilon \psi_i^1 + \dots \quad (3.126)$$

Here, we will only consider the leading order solution, written without the suffix, and express it as a function of the short and the long spatial and temporal variables in the form

$$\psi_i = \psi_i(\zeta(\mathbf{x}, t), \xi, \tau). \quad (3.127)$$

The temporal and spatial derivatives in the original equations may then be written as

$$\begin{aligned} \frac{\partial}{\partial t} &= \frac{\partial \zeta}{\partial t} \frac{\partial}{\partial \zeta} + \varepsilon^{-2} \frac{\partial}{\partial \tau} = \varepsilon^{-1} \frac{\partial Z}{\partial t} \frac{\partial}{\partial \zeta} + \varepsilon^{-2} \frac{\partial}{\partial \tau}, \\ \nabla &= \nabla \zeta \frac{\partial}{\partial \zeta} + \nabla_{\xi} = \varepsilon^{-1} \nabla Z \frac{\partial}{\partial \zeta} + \nabla_{\xi}. \end{aligned} \quad (3.128)$$

When these transformations are introduced into (3.123) one obtains in the vicinity of stoichiometric mixture

$$\begin{aligned} & \rho \frac{\partial \psi_i}{\partial \tau} + \varepsilon^2 \rho \mathbf{v} \cdot \nabla_{\xi} \psi_i + \varepsilon \left[\rho \frac{\partial Z}{\partial t} + \rho \mathbf{v} \cdot \nabla Z \right] \frac{\partial \psi_i}{\partial \zeta} \\ &= \nabla Z \cdot \frac{\partial}{\partial \zeta} \left(\rho D_i \nabla Z \frac{\partial \psi_i}{\partial \zeta} \right) + \varepsilon \nabla_{\xi} \cdot \left(\rho D_i \nabla Z \frac{\partial \psi_i}{\partial \zeta} \right) \\ &+ \varepsilon \nabla Z \cdot \frac{\partial}{\partial \zeta} (\rho D_i \nabla_{\xi} \psi_i) + \varepsilon^2 \nabla_{\xi} \cdot (\rho D_i \nabla_{\xi} \psi_i) + \varepsilon^2 \omega_i. \end{aligned} \quad (3.129)$$

To retain the effect of chemical reactions the chemical source term $\varepsilon^2 \omega_i$ must be of same order as the other leading order terms. We set

$$\varepsilon^2 \omega_i = \Omega_i, \quad (3.130)$$

where Ω_i is of order unity, indicating that the chemical reaction rate ω_i is large. Furthermore, since ∇Z varies only on the long scales, it may be pulled inside the parentheses in the first term on the r.h.s. of (3.129). Introducing this and (3.130) into (3.129) and collecting the leading order terms only, one obtains

$$\rho \frac{\partial \psi_i}{\partial \tau} = \frac{\partial}{\partial \zeta} \left(\rho D_i |\nabla Z|^2 \frac{\partial \psi_i}{\partial \zeta} \right) + \Omega_i. \quad (3.131)$$

If the nondimensional quantity $D_i |\nabla Z|^2$ is rewritten in dimensional form again,

$$\frac{D_i}{D_{st}} |\nabla Z|^2 \left(\frac{\Lambda}{Z'_{st}} \right)^2 = \frac{1}{Le_i} \frac{\chi}{\chi_{st}}, \quad (3.132)$$

the r.h.s. turns out to be of order unity. This should be the case in the asymptotic expansion, thereby justifying the definition of Λ . Since χ varies on the long scales only, the term $D_i |\nabla Z|^2$ can also be taken outside the parentheses in (3.131). Using

$$d\zeta = \varepsilon^{-1} dZ \quad (3.133)$$

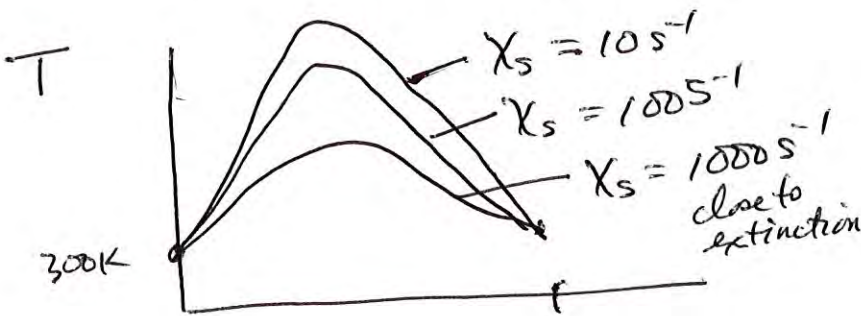
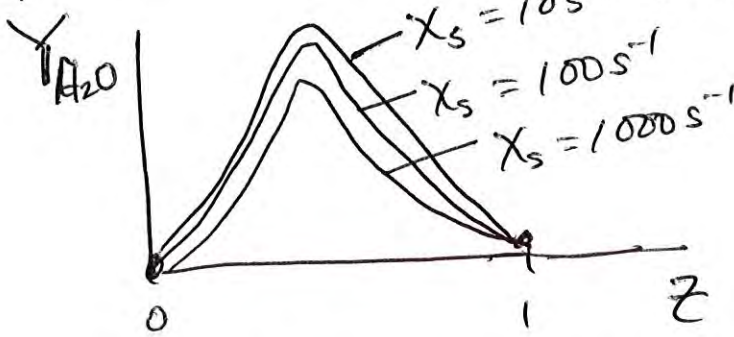
we can rewrite (3.131) in dimensional form again to obtain the classical flamelet equations

flamelet equation (unsteady)	$\rho \frac{\partial \psi_i}{\partial t} = \frac{\rho \chi}{Le_i} \frac{\partial^2 \psi_i}{\partial Z^2} + \omega_i.$	(3.134)
---------------------------------	---	---------

Because of the asymptotic expansion the instantaneous scalar dissipation rate should be that at stoichiometric position, namely χ_{st} defined by (3.30). In one-dimensional flow situations, such as those discussed in Section 3.4, one does not need the asymptotic expansion to obtain flamelet equations like (3.134). This suggests that there is a more general dependence of χ on mixture fraction, as given by (3.47), for instance. We will return to this discussion

two-variable state relations — flamelet eqn solns. for finite chemistry rate to get Y_{CO} , etc

typical solution to flamelet equation



pure ox pure fuel

Realistic State Relations

used in FLUENT and other flamelet models

$$Y_{H2O} = Y_{H2O}(z, X_s)$$

$$T = T(z, X_s)$$

two variable

Conclusion

State relations for a strained C-Flow flame,

=

solve flamelet eqn z is the indep. variable

⇒

(realistic) state relations for $Y_i(z)$
 $T(z)$
 $\rho(z)$

and $w_i(z)$

given X_s assume equal D_i so we can solve z eqn T compute T from adiabatic flame T now we must

allow X_s to vary in turb. flame, so we need to specify the PDF of X_s

Review

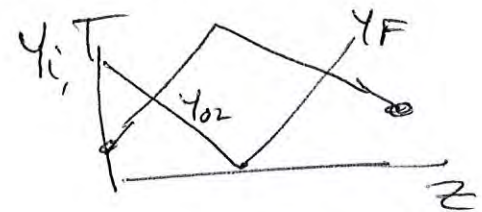
1. solve \bar{z} eqn for $z(x, r)$ in jet

2. ~~use~~ get state relations

to map $z \rightarrow T, Y_i$

at each point

= for ∞ fast (equil chem) = never extinguishes
do not need counterflow solutions



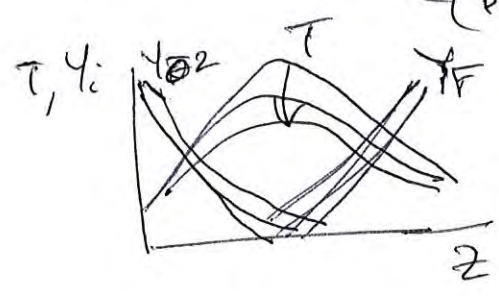
3. get state relations for finite rate chemistry

- extinguishes

- Da controls final temp. - residence time

$$Da = (S_{L,S}^2 / \alpha) / \chi_s$$

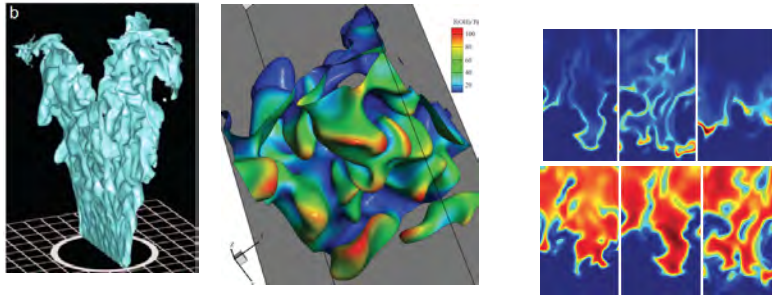
must solve planelet eqn, or CHEMKIN (too slow) for CF plane
(good) (Pitcast)



$$T = T(z, \chi_s)$$

$$Y_{H_2} = Y_{H_2}(z, \chi_s)$$

DNS - 3-D, complex chemistry



Bell, Proc Natl Acad Sciences 102, 29
10006–10011

Aspden J. Fluid Mech 680, 287
Flame in a duct – periodic boundary conditions
Sees broken reactions
Claims to see distributed reactions



13

Background – what does turbulence do ?

Faster mixing - large turbulent diffusivity, shorter flames, smaller combustors

Faster propagation - large turbulent burning velocity avoids blowout

Optimize liftoff height - keep flame away from walls but do not blowout

Reduce Pollutants - less NO_x if velocities are large (for short residence times)
and fuel-air mixing is fast and lean

Avoid growl - combustion oscillations in gas turbines, rockets, due to poor
flame anchoring

Challenge: to model the turbulent reaction rate for
non-premixed, premixed and partially-premixed combustion
what are the best current models, and how good are they ?



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Background

turbulent kinetic energy

$$k = \left(\frac{1}{2}\right) (\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) = \left(\frac{3}{2}\right) \overline{u'^2} \text{ if isotropic}$$

Favre (density-weighted) average

$$\tilde{u} = \frac{\overline{\rho u}}{\bar{\rho}} = \frac{(\overline{\rho + \rho'}) (\overline{u + u'})}{\bar{\rho}} = \bar{\rho} \frac{\bar{u}}{\bar{\rho}} + \frac{\overline{\rho' u'}}{\bar{\rho}} \quad \text{so:}$$

$$\tilde{u} = \bar{u} + \frac{\overline{\rho' u'}}{\bar{\rho}}$$

replacing mean quantities in Navier Stokes Equations with their Favre averages removes all the density fluctuations - this removes one unknown (ρ') but it adds one new unknown: turbulent mass flux: $\overline{\rho' u'}$ which we determine using:

$$\overline{\rho' u'} = -D_T \frac{\partial \bar{\rho}}{\partial x} \quad \text{Prandtl's gradient diffusion assumption}$$



Gradient diffusion assumption - relates Favre avg to time average

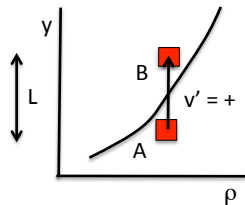
$$\tilde{u} = \bar{u} + \frac{\overline{\rho' u'}}{\bar{\rho}}$$

Favre average gets rid of one unknown (ρ') but introduces another one: $\overline{\rho' u'}$

$$\overline{\rho' u'} = -D_T \frac{\partial \bar{\rho}}{\partial x}$$

$$\overline{\rho' v'} = -D_T \frac{\partial \bar{\rho}}{\partial y}$$

Gradient Diffusion assumption



Suppose $\frac{\partial \bar{\rho}}{\partial y}$ and v' are positive

Small element will carry a low density from A To the higher density region at B. Therefore fluid at B will see a low density fluctuation, thus ρ' is negative at B

So: $\rho' = -L \frac{\partial \bar{\rho}}{\partial y}$ where L = integral scale

Thus $\rho' v' = -L v' \frac{\partial \bar{\rho}}{\partial y}$ taking time average \rightarrow eqn above

We also proved that $D_T = v' L$



Mixing: Turbulent viscosity = diffusivity is large

Since molecular viscosity $\mu / \rho = (\text{speed of sound}) (\text{mean free path})$

Prandtl suggested: $\mu_T / \rho = (u' L) \quad L = \text{integral scale}$

Dissipation rate of TKE $\varepsilon = u'^3 / L$ see turbulence text by Tennekes

Since $u' = k^{1/2}$ then $\varepsilon = k^{3/2} / L$ or $L = k^{3/2} / \varepsilon$

Since we said above $\mu_T = \rho (u') (L)$, then: $\mu_T = c_\mu \bar{\rho} \frac{k^2}{\varepsilon}$

How do we compute k and ε ? Prandtl suggested the k -equation



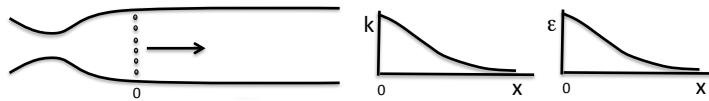
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How to compute turbulence level k and dissipation rate ε ?

$$\bar{\rho} \tilde{u} \frac{\partial k}{\partial x} + \bar{\rho} \tilde{v} \frac{\partial k}{\partial y} = \frac{\partial}{\partial y} \left(\mu_T \frac{\partial k}{\partial y} \right) + \mu_T \left(\frac{\partial \tilde{u}}{\partial y} \right)^2 - \bar{\rho} \varepsilon \quad \text{k-epsilon equations}$$

$$\bar{\rho} \tilde{u} \frac{\partial \varepsilon}{\partial x} + \bar{\rho} \tilde{v} \frac{\partial \varepsilon}{\partial y} = \frac{\partial}{\partial y} \left(\mu_T \frac{\partial \varepsilon}{\partial y} \right) + C_\varepsilon C_D \bar{\rho} k \left(\frac{\partial \tilde{u}}{\partial y} \right)^2 - \frac{C_\varepsilon \bar{\rho} (\varepsilon)^2}{C_D k}$$

convection = diffusion + creation - destruction



Example: Grid in a Wind tunnel $\bar{\rho}, \tilde{u}$ are constant, $\frac{\partial}{\partial y} = 0$ at $x > 0$ behind grid

Given: at $x = 0$ (grid) $k = k_0 = 10 \text{ m}^2/\text{s}^2$ and $\varepsilon = \varepsilon_0 = 1 \text{ (m/s)}^3/\text{m}$ then integrate:

$$\tilde{u} \frac{\partial k}{\partial x} = -\varepsilon \quad \text{and} \quad \tilde{u} \frac{\partial \varepsilon}{\partial x} = -\frac{C_\varepsilon (\varepsilon)^2}{C_D k}$$

Solve on MATLAB

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Non – premixed turbulent flames

Mixture fraction (Z) = mass fraction of H-atoms

$$Z = (Y_H - Y_{H,2}) / (Y_{H,1} - Y_{H,2})$$

Y_H = mass fraction of H atoms contained in all molecules at a point

$Y_{H,1}$ = mass fraction of H atoms entering in stream 1

$Y_{H,2}$ = mass fraction of H atoms entering in stream 2 = 0 for our examples

Ex. Suppose a jet of methane CH₄ is surrounded by a large stream of pure O₂.
Stream 1 = methane, $Y_{H,1} = 4/16 = 0.25$, Stream 2 = O₂, so $Y_{H,2} = 0.0$

At some point P downstream suppose we have 2 moles H₂O and 1 mole CO₂.
At that point,

$$Y_H = \{ 4 \text{ g} / [44 \text{ g} + 2(18 \text{ g})] \} = 0.05$$

$$Z = (Y_H - Y_{H,2}) / (Y_{H,1} - Y_{H,2}) = (0.05 - 0) / [0.25 - 0] = 0.20$$



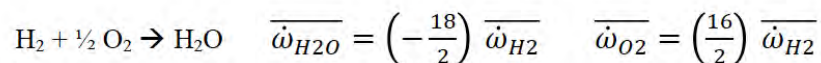
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Conservation equations for, Z, mass fractions of H₂ and O₂

Now consider a planar 2-D jet of H₂ surrounded by a stream of O₂

$$\begin{aligned} \bar{\rho} \tilde{u} \frac{d\bar{Y}_{H_2}}{dx} + \bar{\rho} \tilde{v} \frac{d\bar{Y}_{H_2}}{dy} &= \bar{\rho} D_T \frac{d^2 \bar{Y}_{H_2}}{dy^2} + \overline{\dot{\omega}_{H_2}} \\ \bar{\rho} \tilde{u} \frac{d\bar{Y}_{O_2}}{dx} + \bar{\rho} \tilde{v} \frac{d\bar{Y}_{O_2}}{dy} &= \bar{\rho} D_T \frac{d^2 \bar{Y}_{O_2}}{dy^2} + \overline{\dot{\omega}_{O_2}} \\ \bar{\rho} \tilde{u} \frac{d\bar{Y}_{H_2O}}{dx} + \bar{\rho} \tilde{v} \frac{d\bar{Y}_{H_2O}}{dy} &= \bar{\rho} D_T \frac{d^2 \bar{Y}_{H_2O}}{dy^2} + \overline{\dot{\omega}_{H_2O}} \end{aligned}$$

The rate at which H₂O is formed is related to rate H₂ is consumed:



Inserting these into the above and put in terms of Z to get:

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

Mixture fraction
Conservation eqn
has no source term

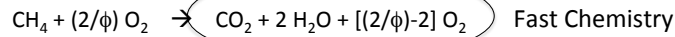


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Flamelet idea: turbulent flame is filled with wrinkled, strained flamelets

State relation - relates mass fraction of O_2 at any point to mixture fraction Z

For our methane mixing into O_2 problem, for lean combustion at any equivalence ratio ϕ :



The gas mixture at any point that resulted from lean combustion must be the mixture in the oval. Assuming fast chemistry. How to relate ϕ to Z ?

For the mixture in the oval, $Z = 4 / [44 + 2(18) + (2/\phi - 2)32] / Y_{H,1}$, where $Y_{H,1} = 0.25$

Solve this for ϕ to get : $\phi = 4Z / (1-Z)$

Now what is Y_{O_2} for the mixture in the oval ? It is

$$Y_{O_2} = [(2/\phi)-2] 32 / \{44 + 36 + [(2/\phi)-2] 32\} = (4 - 4\phi) / (4 + \phi)$$

Insert into this the above formula for ϕ to get:

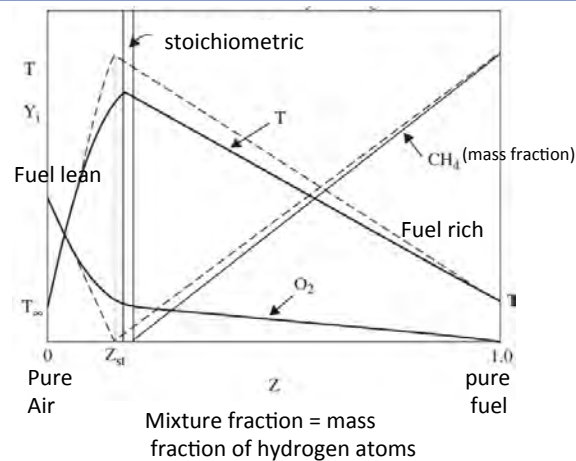
$$Y_{O_2} = (1 - 5Z)$$

(state relation for lean combustion, and Z only varies from 0 to 0.25)



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State relations for unstrained non-premixed flamelets



If you know the instantaneous mixture fraction (Z) at a point P, you use these state relations to look up instantaneous temperature and mass fractions at P



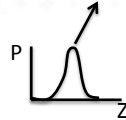
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Probability density function - used to define a mean value

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

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

State relation =
Mass fraction of CO
Conditioned on Z



At each point in the flame, we solve conservation equations to get the mean mixture fraction and variance in mixture fraction $\overline{Z'^2}$

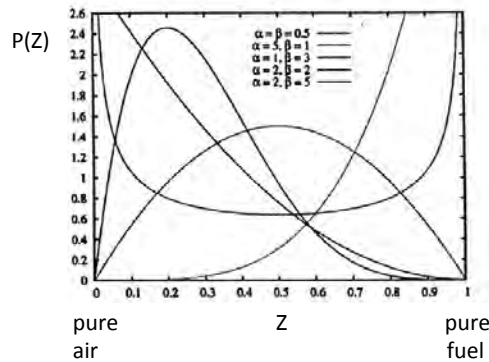
Idea: you only have to solve conservation equations for \bar{Z} and $\overline{Z'^2}$ and use above integral to get other mean values; you avoid solving more conservation equations for each variable



Assume PDF (Z) to be a Beta function for non-premixed flames

$$P(x; \alpha, \beta) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\int_0^1 u^{\alpha-1}(1-u)^{\beta-1} du}$$

here $x = Z =$ mixture fraction
 α and β are related to mean and variance of Z



Turbulent Combustion Concepts

read CANVAS section 2 folder

(Kuo)

A. Favre average \tilde{u} to remove ρ'

define k, ϵ

gradient diffusion hypothesis + Reynolds stress

B. Favre averaged equations, k, ϵ, g eqns

C. Assumed PDF approach

state relations
for instantaneous
 Y_{H_2}

+

$P(\bar{z}, \bar{g})$
+ beta function slope

\Rightarrow

lookup
tables
for
 $\bar{T} = \bar{T}(\bar{z}, \bar{g})$

D. Lockwood-Naguib results
(RANS + equil. chemistry)

Definitions see Kuo, ~~Ch 4.4~~ CANVAS - concepts Eq 4.49

a) Favre-averaged velocity

$$\tilde{u} \equiv \frac{\overline{\rho u}}{\bar{\rho}}$$

"density weighted"
removes ρ' from cons. equations

b) Favre velocity fluctuation

$$u'' \equiv u - \tilde{u}$$

note: $\tilde{u} = \frac{\overline{\rho u}}{\bar{\rho}} = \frac{\overline{(\bar{\rho} + \rho')(u + u')}}{\bar{\rho}} = \frac{\bar{\rho} \bar{u}}{\bar{\rho}} + \frac{\overline{\rho' \bar{u}}}{\bar{\rho}} + \frac{\overline{\bar{\rho} u'}}{\bar{\rho}} + \frac{\overline{\rho' u'}}{\bar{\rho}}$

so $\tilde{u} = \bar{u} + \overline{\rho' u'} / \bar{\rho}$

prove: $\frac{\partial}{\partial x} (\overline{\rho u u}) = \frac{\partial}{\partial x} (\bar{\rho} \tilde{u} \tilde{u})$ Kuo

time averaged term in mom equ

looks same after Favre averaging but \rightarrow do not see ρ' here!

Favre averaging removes ρ' from many places

Favre Averaged Conservation Equations

See Kuo for complex version, see FLUENT, see Lockwood & Naguib CNF 24, 109

Assume: turbulent jet, $p = \text{constant}$, Favre averaged, steady mean, $\frac{\partial}{\partial \theta} = 0$

Seven unknowns: $(\bar{u}, \bar{v}, \bar{Z}, k, \epsilon, g, \bar{\rho})$, seven equations

1. Continuity for radial velocity \bar{v} $\frac{\partial}{\partial z} (\bar{\rho} \bar{u}) + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \bar{v}) = 0$

2. Axial momentum eqn for \bar{u} $\bar{\rho} \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{\rho} \bar{v} \frac{\partial \bar{u}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} v_T \frac{\partial \bar{u}}{\partial r})$

3. Mixture fraction eqn for \bar{Z} $\bar{\rho} \bar{u} \frac{\partial \bar{Z}}{\partial x} + \bar{\rho} \bar{v} \frac{\partial \bar{Z}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \frac{v_T}{\sigma_Z} \frac{\partial \bar{Z}}{\partial r})$

Turbulent kinematic viscosity $v_T = C_D \frac{k^2}{\epsilon}$

4. k equation for k $k = \frac{1}{2} (\overline{u'^2} + \overline{v'^2} + \overline{w'^2})$ turbulent K.E./mass

$$\bar{\rho} \bar{u} \frac{\partial k}{\partial x} + \bar{\rho} \bar{v} \frac{\partial k}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \frac{v_T}{\sigma_k} \frac{\partial k}{\partial r}) + \bar{\rho} v_T \left(\frac{\partial \bar{u}}{\partial r} \right)^2 - \bar{\rho} \epsilon$$

epsilon (ϵ) is the sink term in the k-equation

5. epsilon eqn for ϵ

$$\bar{\rho} \bar{u} \frac{\partial \epsilon}{\partial x} + \bar{\rho} \bar{v} \frac{\partial \epsilon}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \frac{v_T}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial r}) + C_{\epsilon 1} C_D \bar{\rho} k \left(\frac{\partial \bar{u}}{\partial r} \right)^2 - \frac{C_{\epsilon 2}}{C_D} \frac{\bar{\rho} \epsilon^2}{k}$$

6. g equation for scalar fluctuation variance $g = \overline{Z'^2}$

$$\bar{\rho} \bar{u} \frac{\partial g}{\partial x} + \bar{\rho} \bar{v} \frac{\partial g}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \frac{v_T}{\sigma_g} \frac{\partial g}{\partial r}) + C_{g1} \bar{\rho} v_T \left(\frac{\partial \bar{Z}}{\partial r} \right)^2 - \bar{\rho} \bar{\chi}$$

scalar dissipation rate is the sink term in the g-equation:

$$\bar{\chi} = \frac{C_{g2}}{C_D} \left(\frac{\epsilon}{k} \right)$$

7. equation of state for mean density $\bar{\rho}$

$$\bar{\rho} = \int_0^1 \frac{p/R}{T(Z)} P(Z, \bar{Z}, g) dZ$$

need g here

closed set of equations
7 eqns, 7 unknowns

notice no ρ' appears!
look like incompressible laminar eqns

$v \rightarrow v_T$
 $\frac{C_D k^2}{\epsilon} = \frac{(\text{m}^2/\text{s})^2}{\text{m}^2/\text{s}^3} = \text{m}^2/\text{s}$
 $\epsilon = k/t = \frac{\text{m}^2/\text{s}^2}{\text{s}} = \text{m}^2/\text{s}^3$
 $\frac{k}{\epsilon} \cdot t = \frac{\text{m}^2/\text{s}^2}{\text{m}^2/\text{s}^3} \cdot \text{s} = \text{s}$ ✓

need to compute v_T

need to solve k eqn

$g = 0$ no mixing

$C_D = 0.09, C_{\epsilon 1} = 1.45, C_{\epsilon 2} = 0.18, C_{g1} = 2.8, C_{g2} = 0.18$, see Lockwood, CNF 24, 109

Favre Averaged conservation equations (general version found in Kuo)

Notice that density fluctuations ρ' do not appear.

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0 \quad \text{Kuo 4.81}$$

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j) = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (\bar{\tau}_{ij} - \overline{\rho u_i'' u_j''}) \quad \text{Kuo 4.87}$$

$$\underbrace{\frac{\partial}{\partial t} (\bar{\rho} \tilde{h}) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{h} \tilde{u}_j)}_I = \underbrace{\frac{\partial \bar{p}}{\partial t} + \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j}}_{II} + \underbrace{u_j'' \frac{\partial \bar{p}}{\partial x_j}}_{III} + \frac{\partial}{\partial x_j} \underbrace{(-\bar{q}_j - \overline{\rho h'' u_j''})}_{IV} \underbrace{+ \bar{\tau}_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} + \tau_{ij} \frac{\partial u_i''}{\partial x_j}}_V \quad (4.90)$$

Turbulent kinetic energy [per unit mass] = k

$$\tilde{k} \equiv \frac{1}{2} \overline{u_i'' u_i''} = \frac{1}{2} \frac{\overline{\rho u_i'' u_i''}}{\bar{\rho}} \quad \text{Often called } k \text{ without the } (\sim) \quad \text{Kuo 4-104}$$

“k equation”

$$\frac{\tilde{D}}{Dt} \left(\frac{1}{2} \overline{u_i'' u_i''} \right) = - \frac{\partial}{\partial x_k} \overline{u_k'' \left(\frac{1}{2} \overline{\rho u_i'' u_i''} \right)} - \overline{u_i'' \frac{\partial \bar{p}}{\partial x_i}} + \overline{u_i'' \frac{\partial \tau_{ik}'}{\partial x_k}} - \overline{\rho u_i'' u_k'' \frac{\partial \tilde{u}_i}{\partial x_k}} - \frac{1}{2} \overline{\rho u_i'' u_i'' \frac{\partial \tilde{u}_k}{\partial x_k}} \quad (4.106)$$

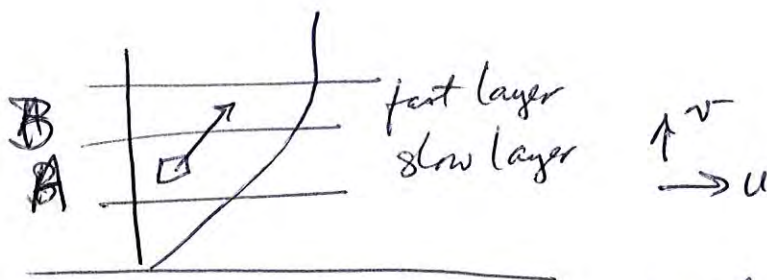
Gradient Diffusion Hypothesis

$$\overline{u'v'} = -\nu_T \frac{\partial \tilde{u}}{\partial y} \quad \text{Reynolds stress}$$

$$\overline{\rho' u'} = -\nu_T \frac{\partial \tilde{p}}{\partial x} \quad \nu_T = D_T = \alpha_T$$

in general:

$$\overline{\phi' u'_i} = -\nu_T \frac{\partial \tilde{\phi}}{\partial x_i} \quad \text{for } \phi = u \text{ or } p$$



suppose eddy jumps from slow layer A up to fast layer B
 then $v' = +$ for this eddy

at location B, $u(t)$ will be



so there will be a $u' = \text{negative}$ due to eddy at B

so at B, eddies with $u' = +$ will have $u' = -$

so $\overline{u'v'} = \text{negative}$

now,

$$|u'| = l \frac{\partial \bar{u}}{\partial y} \quad \text{where } l = \text{mixing distance}$$

$$\text{so } \overline{u'v'} \approx - \overline{\left(l \frac{\partial \bar{u}}{\partial y} \right) \cdot v'} = - \overline{(v'l)} \frac{\partial \bar{u}}{\partial y}$$

$$\text{define } \nu_T = \overline{v'l}$$

$$\text{so } \overline{u'v'} = - \nu_T \frac{\partial \bar{u}}{\partial y} \quad \text{proof}$$

formula for ν_T

$$\text{now } k = \frac{1}{2} (\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) = m^2/s^2$$

$$\epsilon = \frac{dk}{dt} = \frac{m^2/s^2}{s} = \frac{m^2}{s^3}$$

how does $l = \text{mixing length}$ depend on k and ϵ ?

$$l = k^n \epsilon^m$$

solve \rightarrow

$$\text{so } \boxed{l = k^{3/2} / \epsilon}$$

$$\nu_T = \overline{v'l}$$

$$\nu_T = (k^{1/2}) \left(\frac{k^{3/2}}{\epsilon} \right) \cdot c_\mu$$

$$\boxed{\nu_T = c_\mu \frac{k^2}{\epsilon}}$$

$c_\mu = \text{constant}$

Turbulence causes the kinematic viscosity to increase by factor of 100 to 1000!

How are \bar{u} and \tilde{u} related?

you solve eqns for \tilde{u} but what is \bar{u} ?

~~$\tilde{u} = \frac{\rho u}{\bar{\rho}}$~~ so $\rho \tilde{u} = \bar{\rho} u$

$\bar{\rho} \bar{u} = (\bar{\rho} + \rho')(\bar{u} + u')$ $= \bar{\rho} \bar{u} + \bar{\rho}' u'$

$\bar{\rho}' u' = -\cancel{D_T} \frac{\partial \bar{\rho}}{\partial x}$ Grad Diff Hypothesis

so ~~$\tilde{u} = \bar{u} + \frac{D_T}{\bar{\rho}} \frac{\partial \bar{\rho}}{\partial x}$~~

$$\bar{u} = \tilde{u} + \frac{D_T}{\bar{\rho}} \frac{\partial \bar{\rho}}{\partial x}$$

real quantity of interest

compute

after you solve for \tilde{u} and $\bar{\rho}$ which are in your new conservation eqns, use this to back off \bar{u}

- realistically $\frac{\partial \bar{\rho}}{\partial x}$ is small so $\bar{u} \approx \tilde{u}$ in many cases!

k - eqn

derive in Kao P. 231 - see Carwz
Cpt 4

- mom. eqn plug in $p = \bar{p} + p'$, $u = \bar{u} + u'$
~~take time avg of mem. eqn~~ multiply mem. eqn by u_i , take time avg
 subtract from unsteady mem. eqn mult. by u_i
 take time avg of what is left! \rightarrow get ~~the~~ /
 define $(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) / 2 = k$

production of k (turbulence)

in our handout
the production
term is

~~$$\bar{u} \frac{\partial k}{\partial x} = \dots \bar{\nu} \frac{\partial \bar{u}}{\partial r}$$~~

k/second

rate of k/sec produced = $\nu_T \left(\frac{\partial \bar{u}}{\partial r} \right)^2$

turbulence is
created where
there are
mean gradients
shear layer, b.l.s

destruction
of k
(k/sec)

$$= \epsilon = \nu \frac{\partial u_i'}{\partial x_j'} \frac{\partial u_i'}{\partial x_j'}$$

model it as $\epsilon =$ from ϵ eqn

g-equation = conservation of scalar fluctuations

Why? to determine $\bar{T} = \int_0^1 T(f) P(f) df$
 state relation (known) \uparrow beta function \uparrow

but $P(f)$ has a mean (\bar{f}) and a variance (g) that must be known at every (x, y, z) point to compute \bar{T}

\rightarrow use \bar{f} equation to get \bar{f} (we derived in class)

\rightarrow need g-equation to g

$$g \equiv \overline{f'^2}$$

$\bar{\chi} =$ sink term in the g equation

Derive the "g-equation" scalar dissipation rate

- 1 write the unsteady conservation of conserved scalar f
- 2 write the Favre-avgd. conservation eqn of conserved scalar f
- 3 subtract, square the result and take the time average

Kuo, p. 454 shows that:

exact g-equation
Kuo (7-175)

$$\underbrace{\rho u_k \frac{\partial g}{\partial x_k}}_{\text{convection of scalar fluctuations}} = \underbrace{-2\rho u_k'' \frac{\partial \bar{f}}{\partial x_k}}_{\text{production of scalar fluct. by mean grad. (source)}} - \underbrace{\frac{2}{\rho} \rho u_k'' \frac{\partial \bar{f}}{\partial x_k}}_{\text{diffusion of scalar fluct.}} - \underbrace{2\rho D \left(\frac{\partial \bar{f}''}{\partial x_k} \right)^2}_{\text{p*scalar dissipation rate (-p\bar{\chi}) (sink)}}$$

$$\bar{\chi} \equiv 2D \left[\left(\frac{\partial \bar{f}}{\partial x} \right)^2 + \left(\frac{\partial \bar{f}}{\partial y} \right)^2 + \left(\frac{\partial \bar{f}}{\partial z} \right)^2 \right]$$

using gradient diffusion modeling assumption, for jet geometry:

$$\bar{\rho} \tilde{u} \frac{\partial g}{\partial x} + \bar{\rho} \tilde{v}_r \frac{\partial g}{\partial r} = -\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r \mu_t}{\sigma_g} \frac{\partial g}{\partial r} \right) + C_{g1} \mu_t \left(\frac{\partial \tilde{f}}{\partial r} \right)^2 - C_{g2} \bar{\rho} \frac{g \epsilon}{k}$$

diffusion
production
scalar dissipation

The "g-equation"
 (not in Kao)

Lockwood + Naqib
 Equation (11)

(C+F 24,
 p. 109, 1975)

here he assumes that

$$-2 \bar{\rho} D \left(\frac{\partial \tilde{f}''}{\partial x_k} \right)^2 = -2 \bar{\rho} \bar{D} \overline{\left(\frac{\partial \tilde{f}''}{\partial x_k} \right)^2} = -\bar{\rho} \bar{\chi}$$

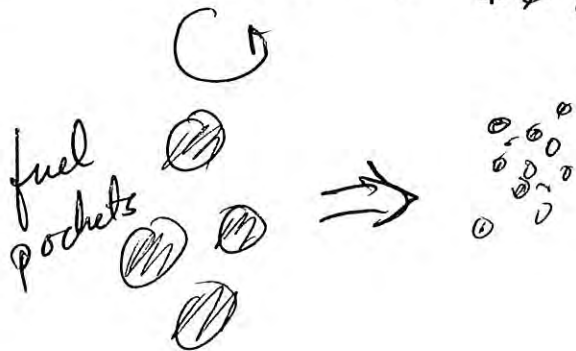
$$= -C_{g2} \bar{\rho} \frac{g \epsilon}{k}$$

ie that $\bar{\chi} = C_{g2} g \left(\frac{\epsilon}{k} \right)$ assumption

scalar dissipation (s⁻¹)
 non-dim.
 $\epsilon =$ rate of k dissipated / sec
 $\epsilon/k = (s^{-1})$

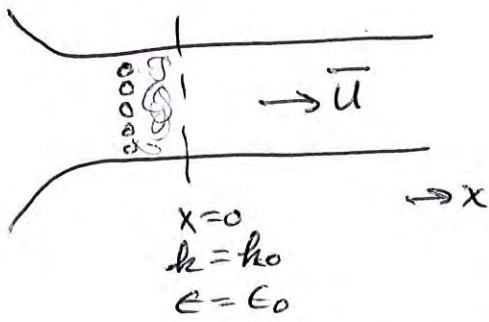


eddies (velocity fluctuations) get smaller + viscosity destroys them



fuel pockets (scalar fluctuations) get smaller + viscosity destroys them

Example #1



solve $k-\epsilon$ eqns for grid turbulence

given - wind tunnel with grid to create turbulence k_0 at $x=0$

$\rho = \text{constant}$, stationary $\frac{\partial}{\partial t} = 0$

$$k \equiv \overline{u'^2} + \overline{v'^2} + \overline{w'^2} \quad \frac{\partial}{\partial y} = 0$$

k eqn becomes

$$\cancel{\rho \bar{u}} \frac{\partial k}{\partial x} + \cancel{\rho \bar{v}} \frac{\partial k}{\partial y} = \cancel{\frac{\partial}{\partial y}} \left(\cancel{\rho \bar{v}_T} \frac{\partial k}{\partial y} \right) + \cancel{\frac{\partial}{\partial y}} \left(\cancel{\rho \bar{v}_T} \frac{\partial \bar{u}}{\partial y} \right) - \cancel{\rho} \epsilon$$

(a) so $\boxed{\frac{dk}{dx} = -\frac{\epsilon}{\bar{u}}}$

ϵ eqn $\rho \bar{u} \frac{\partial \epsilon}{\partial x} + \rho \bar{v} \frac{\partial \epsilon}{\partial y} = \frac{\partial}{\partial y} \left(\rho \bar{v}_T \frac{\partial \epsilon}{\partial y} \right) + c_{\epsilon 1} \rho \bar{v}_T k \left(\frac{\partial \bar{u}}{\partial y} \right)^2 - \frac{c_{\epsilon 2}}{C_D} \rho \bar{v}_T \frac{\epsilon^2}{k}$

(b) so $\boxed{\frac{d\epsilon}{dx} = -\frac{c_{\epsilon 2} \epsilon^2}{C_D \bar{u} k}}$, $\frac{c_{\epsilon 2}}{C_D} = 2$

solve analytically by dividing (a) by (b):

$$\frac{dk/dx}{d\epsilon/dx} = \frac{-(\epsilon/\bar{u})}{-(2/\bar{u})(\epsilon^2/k)} \Rightarrow \frac{dk}{d\epsilon} = \frac{\epsilon^{-1} k}{2} \Rightarrow 2 \frac{dk}{k} = \frac{d\epsilon}{\epsilon}$$

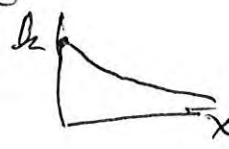
so $2 \ln k = \ln \epsilon + \text{const}$ or $\ln k^2 = \ln \epsilon + \text{const}$
 $\therefore k^2 = A \epsilon$ but $k_0^2 = A \epsilon_0$ at $x=0$ so $A = k_0^2 / \epsilon_0$

and $k^2 = (k_0^2 / \epsilon_0) \epsilon$ at all x . plug this in eqn (a)

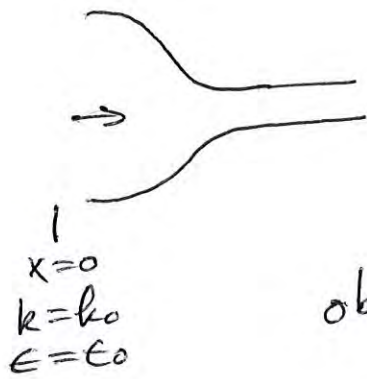
$$\frac{dk}{dx} = -\frac{1}{\bar{u}} k^2 \left(\frac{\epsilon_0}{k_0^2} \right) \Rightarrow \int_{k_0}^k \frac{dk}{k^2} = \left(-\frac{1}{\bar{u}} \frac{\epsilon_0}{k_0^2} \right) \int_{x=0}^x dx$$

$$\boxed{k(x) = \left(\frac{\epsilon_0}{k_0^2} \frac{x}{\bar{u}} + k_0^{-1} \right)^{-1}}$$

$$\boxed{\epsilon(x) = \frac{\epsilon_0}{k_0^2} \left(\frac{\epsilon_0}{k_0} \frac{x}{\bar{u}} + k_0^{-1} \right)}$$



Example #2 Reduction of turbulence in nozzle



subsonic nozzle
constant density

k_0, ϵ_0 given
at $x=0$

$$\dot{m} = \bar{\rho} \bar{u} A$$

$$\frac{dA}{dx} = \text{negative so } \frac{d\bar{u}}{dx} = \text{positive}$$

$$\partial/\partial y = 0$$

observe = nozzle causes k to decrease rapidly
good - test section is almost laminar

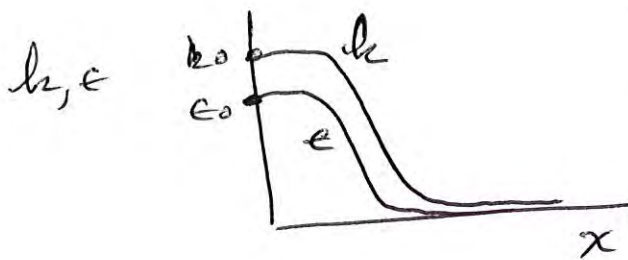
$$\bar{\rho} \bar{u} \frac{dk}{dx} = + \bar{\rho} \nu_T \left(\frac{d\bar{u}}{dx}\right)^2 - \bar{\rho} \epsilon$$

$$\bar{\rho} \bar{u} \frac{d\epsilon}{dx} = C_{\epsilon 1} C_D \bar{\rho} k \left(\frac{d\bar{u}}{dx}\right)^2 - \frac{C_{\epsilon 2}}{C_D} \bar{\rho} \frac{\epsilon^2}{k}$$

plug in: $\nu_T = C_D k^2/\epsilon$ and $\frac{d\bar{u}}{dx} = \frac{-\dot{m}}{\bar{\rho} A^2} \frac{dA}{dx}$ } given

solve on MATLAB - get

- very rapid reduction of k and ϵ in x direction



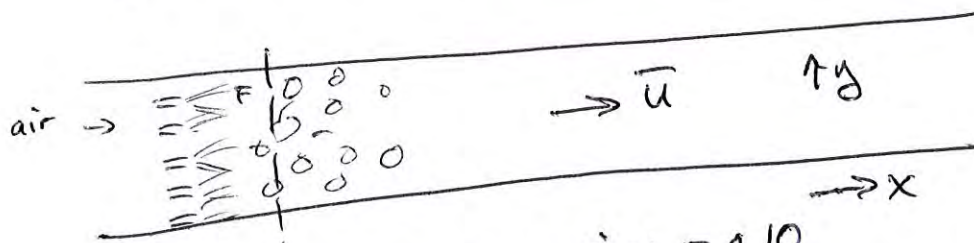
the $d\bar{u}/dx$ term causes
a more rapid reduction
of k

Example #3

Decay of scalar fluctuations

(g) in wind tunnel

suppose we have many small fuel jets and air jets at $x=0$
 downstream is a constant velocity (\bar{u}) wind tunnel
 density = constant



$$\frac{\partial}{\partial y} = 0$$

$x=0 \quad g = g_0 = \text{given} = 0.10$

$$g \equiv \overline{z'^2}$$

= variance in mixture fraction fluctuations

what distance is required to "mix" - to decrease g to 0.05

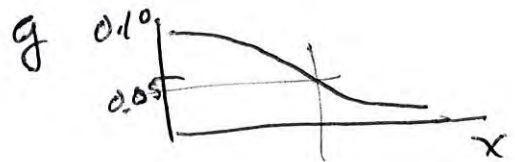
$$\bar{\rho} \bar{u} \frac{\partial g}{\partial x} + \bar{\rho} \bar{v} \frac{\partial g}{\partial y} = \frac{\partial}{\partial y} \left(\bar{\rho} \frac{\nu_T}{\sigma_g} \frac{\partial g}{\partial y} \right) + C_{g1} \bar{\rho} \nu_T \left(\frac{\partial \bar{z}}{\partial y} \right)^2 - \rho \bar{\chi} \quad \text{where } \bar{\chi} = \frac{C_{g2} \epsilon}{\rho D T}$$

so

$$\bar{u} \frac{dg}{dx} = - \frac{C_{g2} \epsilon}{\rho D T}$$

combine this with k_2 and ϵ eqns and solve for $g(x)$

FLUENT does this.

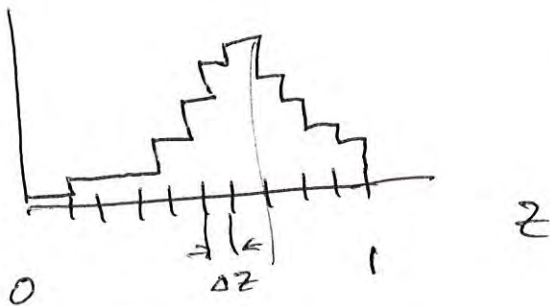


PDF of z

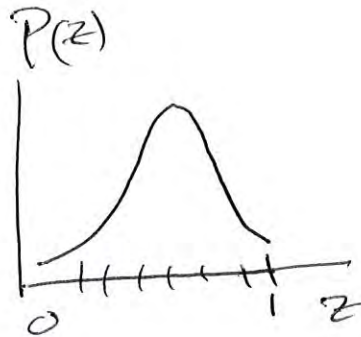


sample t - ensemble

samples
in each
bin



normalize
so
area =
= 1



Prob of z between z and $z + \Delta z = \frac{\text{\# samples in each bin}}{\text{total samples}}$

$$\int_a^b P(z) dz$$

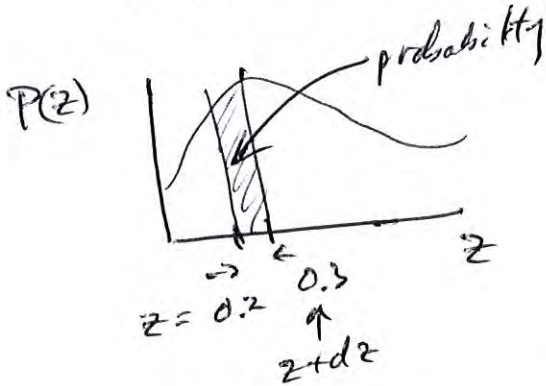
if $dz =$ larger
have more
samples

$$\text{area} = \int_0^1 P d(z) = 1$$

PDF approach - Moments

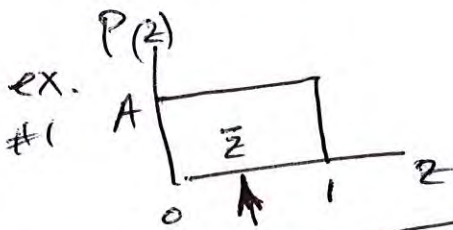
$P(z)$ = PDF = prob. density function of z = histogram

$P(z) dz$ = prob. that z lies between z and $z+dz$

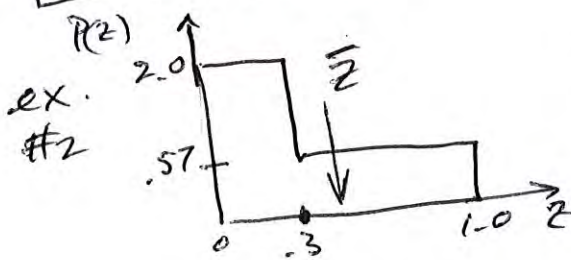


$$P(z) = A$$

$$\int_0^1 P(z) dz = 1 \quad \text{so} \quad A \int_0^1 dz = 1 \quad A = 1$$



$$\bar{z} = \int_0^1 z P(z) dz = \int_0^1 z \cdot 1 dz = \frac{z^2}{2} \Big|_0^1 = \frac{1}{2} \quad \text{as expected}$$



$$\int_0^1 P(z) dz = \int_0^{0.3} 2.0 dz + \int_{0.3}^{1.0} 0.57 dz = 0.6 + 0.4 = 1.0$$

$$\bar{z} = \int_0^1 z P(z) dz = \int_0^{0.3} (2.0z) dz + \int_{0.3}^{1.0} (0.57z) dz$$

$$\bar{z} = z^2/2 \Big|_0^{0.3} \cdot 2 + \frac{z^2}{2} \Big|_{0.3}^1 \cdot 0.57 = 0.35$$

$$\bar{z}^2 = \int_0^1 (z - \bar{z})^2 P(z) dz = \int_0^{0.3} (z - 0.35)^2 2.0 dz + \int_{0.3}^1 (z - 0.35)^2 0.57 dz$$

$$\overline{z'^2} = \int_0^1 (z - \bar{z})^2 P(z) dz$$

$$= \int_0^{0.3} (z - 0.35)^2 (2.0) dz + \int_{0.7}^{1.0} (z - 0.35)^2 0.57 dz$$

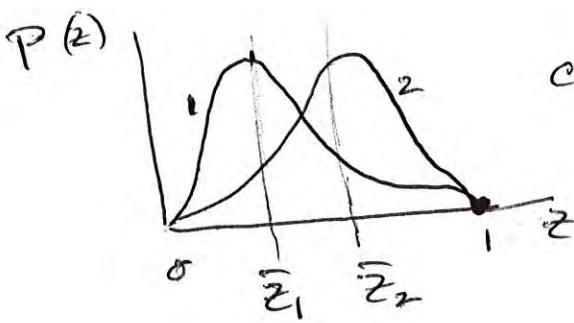
Assumed PDF shape approach

assume PDF is a Beta function = $P(z)$

$$P(z) = \text{Beta} \left(z, \bar{z}, \overline{z'^2} \right)$$

\uparrow mean \uparrow variance

$$\overline{z'^2} = g$$



case 1 has smaller mean than case 2
both have about same variance

$$\text{standard deviation} = \text{r.m.s.} = \sqrt{\text{variance}}$$

Both are Beta functions
pure zero fuel, zero pure air

Example

Bimodal PDF
premixed flame

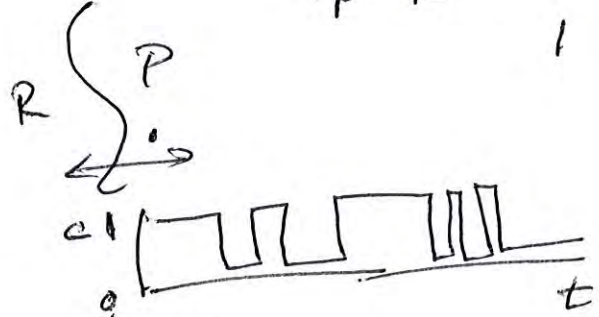
$c = \text{non-dim Temperature} = \text{reactedness}$



$$c = \frac{T - T_R}{T_P - T_R} = 0 \text{ unburned reactants}$$

1 burned products

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



$$\int_0^1 P(c) dc = 1 = A \int_0^1 \delta(c) dc + B \int_0^1 \delta(c-1) dc$$

$$1 = A + B \quad \therefore B = 1 - A \quad A = 1 - B$$

what is \bar{c} ? $\bar{c} = \int_0^1 c P(c) dc = c A \Big|_{c=0} + c B \Big|_{c=1}$

$$\bar{c} = B$$

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

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

↑
(mean)

Variance

$$\bar{p} = \int_0^1 \bar{p}(c) P(c) dc = \int \frac{p}{RT} P(c) dc$$

$p = \text{const}$
 $R = \text{const}$

Q: what is $T(c)$? $T = (T_P - T_R)c + T_R$ from definition of c

$$\bar{p} = \frac{P}{R} \int_0^1 \frac{1}{(T_P - T_R)c + T_R} [A S(c) + B S'(c)] dc$$

$$= \frac{P}{R} \left[\frac{A}{(T_P - T_R)c + T_R} \right]_{c=0} + \frac{P}{R} \left[\frac{B}{(T_P - T_R)c + T_R} \right]_{c=1}$$

$$= \frac{P}{R T_R} A + \frac{P}{R T_P} B = \rho_R \overset{\uparrow}{1-\bar{c}} A + \rho_P \overset{\uparrow}{\bar{c}} B$$

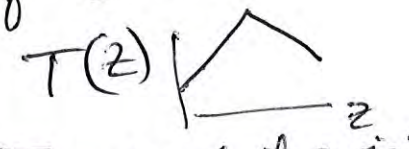
$$\begin{aligned} \checkmark \bar{c} = 0 \quad \rho = \rho_R \\ \checkmark \bar{c} = 1 \quad \rho = \rho_P \quad \checkmark \end{aligned}$$

$$\boxed{\bar{p} = \rho_R (1 - \bar{c}) + \rho_P \bar{c}}$$

(a) one independent variable (z) has PDF that is defined by its mean + its variance \bar{z}, \bar{z}'^2 (no strain, no dissipation rate)

$$\bar{T}(\bar{z}, \bar{z}'^2) = \int_0^1 T(z) P(z, \bar{z}, \bar{z}'^2) dz$$

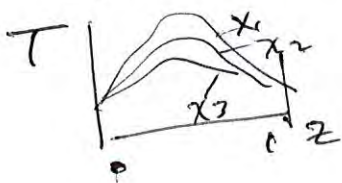
- when you integrate the z in the integral disappears so \bar{T} is not a function of z , only \bar{z} and \bar{z}'^2

- if you provide values of \bar{z} and \bar{z}'^2 and the state relation  you then can compute \bar{T} at that point in space

(b) two independent variables (z, χ_s) now include strained flamelets

$$\bar{T}(\bar{z}, \bar{z}'^2, \bar{\chi}_s, \bar{\chi}_s'^2) =$$

$$\int_{10/s}^{1020/s} \int_0^1 T(z, \chi_s) P_1(z, \bar{z}, \bar{z}'^2) \cdot P_2(\chi_s, \bar{\chi}_s, \bar{\chi}_s'^2) dz d\chi_s$$



Beta function with mean + variance

log normal function with mean + variance

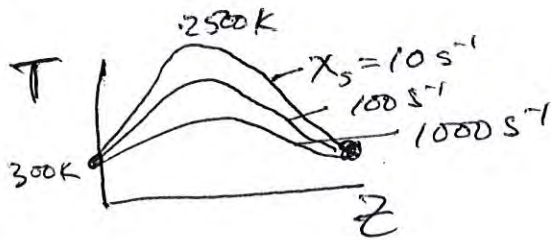
$$\bar{T}(\bar{z}, g, \bar{\chi}_s, \bar{\chi}_s'^2) = \int_0^1 \int_0^\infty T(z, \chi_s) P_1(z, \bar{z}, g) P_2(\chi_s, \bar{\chi}_s, \bar{\chi}_s'^2) dz d\chi_s$$

at each point P, need conservation equations for

$$(\bar{z}, g = \bar{z}'^2, \bar{\chi}_s, \bar{\chi}_s'^2)$$

also assume $P_1 =$ Beta function $P_2 =$ Log normal function
integrate over z and χ_s so z and χ_s dropout (dummy variables)

insert $T(z, \chi_s) =$ state relation for instantaneous T, z and χ_s



two variable state relation (z, χ_s)

∴ given the four numbers in () and state relations
I can compute \bar{T} at a point

\bar{z} comes from \bar{z} conservation eqn

g comes from g conservation eqn

$\bar{\chi}_s$ comes from FLUENT modeling eqn:

$$\bar{\chi}_s = C_x \frac{e g}{k}$$

$$\bar{\chi}_s'^2 = 0$$

Derive

1) k-eqn (TKE)

- \bar{u} • x-mom unsteady
- \bar{v} • y-mom "
- \bar{w} • z-mom "
- $-\bar{u}$ • x-mom steady (time avgd)
- $-\bar{v}$ • y-mom "
- $-\bar{w}$ • z-mom "slit"

→ k eqn.

$$\epsilon \equiv \nu \overline{\frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j}}$$

2) ϵ -eqn Tenenches p-87

- take $\frac{\text{Curl}}{\nabla \times}$
- $\nabla \times$ (x-mom eqn, unsteady)
 - $\nabla \times$ (y-mom " ")
 - $\nabla \times$ (z-mom " ")
 - $-\nabla \times$ (x-mom, time avgd)
 - $-\nabla \times$ (y-mom " ")
 - $-\nabla \times$ (z-mom " ")

$$\rightarrow \frac{\partial u}{\partial x}$$

$$\frac{\partial u'}{\partial x}$$

$$\frac{\partial \bar{u}}{\partial x}$$

vector eqn

→ ~~unsteady~~ take dot product of

$\bar{w}'_z = \text{vertical fluct.}$

→ scalar eqn for $\frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j}$

- take time avg

Derive turbulent kinetic energy (TKE) equation

see Tennekes p. 63, Pope 125, 133, Hinze p. 65

1. write unsteady momentum equations, multiply by u_i
2. write time-averaged momentum equations, multiply by $-\bar{u}_i$
3. add and take time average

$$\begin{aligned} & \downarrow \text{first term} \quad \downarrow \text{second term} \\ & u_i \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \dots \right) \\ & -\bar{u}_i \left(\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = \dots \right) \end{aligned}$$

add and take time average.

ex. lets do the first term; it is

$$\begin{aligned} \overline{u_i \frac{\partial u_i}{\partial t}} - \overline{\bar{u}_i \frac{\partial \bar{u}_i}{\partial t}} &= \overline{(\bar{u}_i + u_i') \left(\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial u_i'}{\partial t} \right)} - \overline{\bar{u}_i \frac{\partial \bar{u}_i}{\partial t}} \\ \uparrow \text{insert } u_i &= \bar{u}_i + u_i' \\ &= \overline{\bar{u}_i \frac{\partial \bar{u}_i}{\partial t}} + \overline{\bar{u}_i \frac{\partial u_i'}{\partial t}} + \overline{u_i' \frac{\partial \bar{u}_i}{\partial t}} + \overline{u_i' \frac{\partial u_i'}{\partial t}} - \overline{\bar{u}_i \frac{\partial \bar{u}_i}{\partial t}} \\ &= \overline{u_i' \frac{\partial u_i'}{\partial t}} = \frac{\partial}{\partial t} \left(\frac{1}{2} \overline{u_i' u_i'} \right) = \boxed{\frac{\partial k}{\partial t}} \end{aligned}$$

let's do the second term (for HW)

$$\begin{aligned}
 & \overline{u_i u_j \frac{\partial u_i}{\partial x_j}} - \bar{u}_i \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = (\bar{u}_i + u_i') (\bar{u}_j + u_j') \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial u_i'}{\partial x_j} \right) - \bar{u}_i \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} \\
 & \text{take time average} \\
 & = \bar{u}_i \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \overline{u_i' \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j}} + \bar{u}_i \bar{u}_j \left(\frac{\partial u_i'}{\partial x_j} \right) + \overline{u_j' (u_i' \frac{\partial u_i'}{\partial x_j})} \\
 & + \bar{u}_i \overline{u_j' \left(\frac{\partial \bar{u}_i}{\partial x_j} \right)} + \overline{(u_i' u_j') \frac{\partial \bar{u}_i}{\partial x_j}} + \bar{u}_i \overline{u_j' \left(\frac{\partial u_i'}{\partial x_j} \right)} \quad \star \\
 & + \overline{(u_i' u_j') \frac{\partial u_i'}{\partial x_j}} - \overline{\bar{u}_j \frac{\partial u_i'}{\partial x_j}}
 \end{aligned}$$

the \star term is:

$$\bar{u}_j \frac{\partial u_i'}{\partial x_j} = \bar{u}_j \frac{\partial}{\partial x_j} \left(\frac{1}{2} \overline{u_i' u_i'} \right) = \frac{\partial k}{\partial x_j} \bar{u}_j$$

$$\text{second term} = \underbrace{\bar{u}_j \frac{\partial k}{\partial x_j}}_{\text{convection of } k} + \bar{u}_i \overline{u_j' \frac{\partial u_i'}{\partial x_j}} + \overline{u_i' u_j'} \underbrace{\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)}_{\sim \text{mean strain rate}}$$

\uparrow
 Reynolds stress

we see that the TKE is produced

by a (Reynolds stress) \times (mean strain rate)

Result is Reynolds avg'd TKE eqn "k-equation"
 (NOT THE FINAL FORM) - EXACT FORM

$$\frac{\partial k}{\partial t} + \bar{u}_j \frac{\partial k}{\partial x_j} = -\frac{2}{\rho} \left(\frac{1}{\rho} \overline{u_j' p'} + \frac{1}{2} \overline{u_i' u_i' u_j'} - 2\nu \overline{u_j' s_{ij}'} \right)$$

convection p-work turb. diffusion molec. diffusion

$$- \overline{u_i u_j} \bar{s}_{ij} - 2\nu \overline{s_{ij}' s_{ij}'}$$

production viscous dissipation

Tennekes p. 63 $\rho = \text{const}$

exact TKE eqn (see next page)

production of k ("turbulence") = $\frac{\text{Reynolds stress}}{\rho} \times \text{mean strain rate } \bar{s}_{ij}$

Reynolds stress = $-\rho \overline{u_i u_j}$

mean strain rate $\bar{s}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$ $s_{ij}' = \frac{1}{2} \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right)$

dissipation rate = (molecular viscosity) * (fluctuating strain rate squared)

dissipation rate $\epsilon = 2\nu \overline{s_{ij}' s_{ij}'}$

we can show that

(molecular diffusion term) + (turbulent diffusion term) = $\frac{\partial}{\partial x_j} \left[(\nu + \nu_T) \frac{\partial k}{\partial x_j} \right]$

define $\nu_T = -1/2 \overline{u'_i u'_i u'_j} / \left(\frac{\partial k}{\partial x_j} \right)$

$\epsilon = -2 \nu \overline{s'_{ij} s'_{ij}}$

TKE becomes

$$\frac{\partial k}{\partial t} + \bar{u}_j \frac{\partial k}{\partial x_j} = \overline{u'_i u'_j} \left(\frac{\partial \bar{u}_i}{\partial x_j} \right) - \epsilon + \frac{\partial}{\partial x_j} \left[(\nu + \nu_T) \frac{\partial k}{\partial x_j} \right]$$

zero if stationary convection

Tennekes, p. 63
Hinze p. 65

production = $\overline{u'_i u'_j} \left(\frac{\partial \bar{u}_i}{\partial x_j} \right)$
(Re stress) x (mean vel. grad)

$-\frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \overline{u'_j p'} \right)$
pressure work (normally small)

if stationary, neglect pressure work, constant density

$$\bar{u}_j \frac{\partial k}{\partial x_j} = \overline{u'_i u'_j} \left(\frac{\partial \bar{u}_i}{\partial x_j} \right) - \epsilon + \frac{\partial}{\partial x_j} \left[(\nu + \nu_T) \frac{\partial k}{\partial x_j} \right]$$

convection production dissip diffusion

Turbulent Kinetic Energy Eqn

Tennekes p. 63
Hinze p. 65

Kuo

TKE

3.3.5 Turbulence-Kinetic-Energy Equation

For $i = j$, Eq. (7-93) becomes the turbulence-kinetic-energy equation:

$$\underbrace{\frac{D}{Dt} \left(\frac{1}{2} \overline{\rho u_i'' u_i''} \right)}_I + \underbrace{\frac{\partial}{\partial x_k} \overline{u_k'' \left(\frac{1}{2} \rho u_i'' u_i'' \right)}}_II = - \underbrace{\overline{u_i'' \frac{\partial p}{\partial x_i}}}_{III} + \underbrace{\overline{u_i'' \frac{\partial \tau_{ik}'}{\partial x_k}}}_{IV} - \underbrace{\frac{1}{2} \overline{\rho u_i'' u_k''} \frac{\partial \bar{u}_i}{\partial x_k}}_V$$

(7-94)

The physical meanings of the terms of Eq. (7-94) are as follows:

- I: $\frac{D}{Dt} \left(\frac{1}{2} \overline{\rho u_i'' u_i''} \right)$ Rate of change of kinetic energy of turbulence
- II: $\frac{\partial}{\partial x_k} \overline{u_k'' \left(\frac{1}{2} \rho u_i'' u_i'' \right)}$ Kinetic energy of fluctuations convected by the fluctuations (i.e., diffusion of fluctuation energy)
- III: $\overline{u_i'' \frac{\partial p}{\partial x_i}}$ Work due to turbulence
- IV: $\overline{u_i'' \frac{\partial \tau_{ik}'}{\partial x_k}}$ Work of viscous stresses due to fluctuation motion
- V: $-\overline{\rho u_i'' u_k''} \frac{\partial \bar{u}_i}{\partial x_k} - \overline{\rho u_i'' u_i''} \frac{\partial \bar{u}_k}{\partial x_k}$ Product of turbulent stress and mean rate of strain: production of turbulent energy

3.3.6 Species Conservation Equation

The species conservation equation based upon the Favre averaging can be shown to have the following form:

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_k) + \frac{\partial}{\partial x_i} (\bar{\rho} \bar{Y}_k \bar{u}_i) = \frac{\partial}{\partial x_i} \left[\mathcal{D} \bar{\rho} \frac{\partial \bar{Y}_k}{\partial x_i} - \overline{\rho Y_k'' u_i''} \right] + \frac{\partial}{\partial x_i} \overline{\mathcal{D} \rho \frac{\partial Y_k''}{\partial x_i}} + \bar{\omega}_k \quad (7-95)$$

It will be useful for the reader to determine the physical meanings of the terms in the above equation.

3.4 Effect of Vorticity on Turbulent Flames

The vorticity equation can be obtained by taking the curl of the momentum equation. The reason that we are interested in the vorticity equation is the

Turbulent kinetic energy equation (k eqn)

- exact form derived in Hinze Turbulence

multiply	u	times	x-momentum eqn (unsteady)
	v	times	y-mom
	w	times	z-mom
	\bar{u}	times	x-mom, (time avgd)
	\bar{v}	times	y-mom
	\bar{w}	times	z-mom
add + take time average:			

exact form

$$\frac{D}{Dt} \left(\frac{1}{2} \rho \overline{u_i'' u_i''} \right) = - \frac{\partial}{\partial x_j} \left(\overline{u_j'' \frac{1}{2} \rho u_i'' u_i''} \right) - \overbrace{u_i'' \frac{\partial p}{\partial x_i}}^{\text{"sink"}} + \overbrace{u_i'' \frac{\partial \tau_{ik}}{\partial x_k}}^{\text{"source"}} - \rho \overline{u_i'' u_k''} \frac{\partial u_i}{\partial x_k}$$

rate of change of TKE/vol = diffusion of TKE by turbulent velocity fluctuations + work/sec per volume done by pressure forces = work/sec vol due to molecular viscosity production of TKE (ie velocity fluctuations) due to mean flow gradients

as follows element

Kuo p. 427
Hinze p. 65

Tennekes + Lumley p. 63

$$k \equiv \frac{\overline{u''^2} + \overline{v''^2} + \overline{w''^2}}{2}$$

Kuo p. 445

In the k-ε model, this complex relation for k is simplified to:

Modelled form

$$\rho \bar{u} \frac{\partial k}{\partial x} + \rho \bar{v} \frac{\partial k}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu_t \frac{\partial k}{\partial r} \right) - \underbrace{\bar{\rho} \epsilon}_{\text{sink}} + \underbrace{\mu_t \left(\frac{\partial \bar{u}}{\partial r} \right)^2}_{\text{production term}}$$

convection of k diffusion of k (dissipation of k = $-C_D \rho^2 k^2 / \mu_t$)

where $k = \frac{\overline{u''^2} + \overline{v''^2} + \overline{w''^2}}{2} = \left(\frac{\text{meters}}{\text{sec}} \right)^2 = \frac{\text{KE}}{\text{mass}}$

Lockwood Eqn 3

The dissipation rate (ϵ) equation

$$\epsilon \equiv \nu \overline{\frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j}} = \nu \left[\overline{\left(\frac{\partial u'}{\partial x}\right)^2} + \overline{\left(\frac{\partial u'}{\partial y}\right)^2} + \overline{\left(\frac{\partial u'}{\partial z}\right)^2} + \overline{\left(\frac{\partial v'}{\partial x}\right)^2} + \dots \right]$$

Kuo
p. 428

RELATED to VORTICITY FLUCTUATIONS

$\epsilon = 15 \nu \overline{\left(\frac{\partial u'}{\partial x}\right)^2}$ for isotropic turbulence

define Taylor microscale

$$\lambda_T = \sqrt{\overline{u'^2} / \overline{\left(\frac{\partial u'}{\partial x}\right)^2}}$$

$$\therefore \epsilon = 15 \nu \overline{u'^2} / \lambda_T^2$$

isotropic turbulence

$$\lambda_T = 7.01 \left(\frac{\overline{u'^2}}{\nu}\right)^{-1/2}$$

but for non-isotropic turbulence:

Derive ϵ eqn (exact form)

Kuo
Tennekes p. 87

- take curl of mom. eqns to derive unsteady vorticity eqn
- take dot product of w_j with unsteady vorticity eqn $\Rightarrow \overline{w_j'^2}$
- take dot product of w_j with steady vorticity eqn $\Rightarrow \overline{w_j^2}$

$\overline{w_j'^2} = \overline{w_j^2} - \overline{w_j^2} \Rightarrow$ subtract last two eqns to get:

exact form

$$\frac{D}{Dt} \left(\frac{\overline{w_i'^2}}{2} \right) = - \overline{u_j' w_i'} \frac{\partial \overline{w_i}}{\partial x_i} - \frac{1}{2} \frac{\partial}{\partial x_j} \overline{u_j' w_i'^2} + \overline{w_i w_j} \overline{S_{ij}} - \nu \overline{\left(\frac{\partial w_i'}{\partial x_j}\right)^2}$$

rate of change of vorticity fluct. = production of vort. fluct. + diffusion of vort. fluct. + vortex stretching + dissipation of vort. fluct.

model this as:

$$\bar{\rho} \tilde{u} \frac{\partial \epsilon}{\partial x} + \bar{\rho} \tilde{v}_r \frac{\partial \epsilon}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial r} \right) + C_{\epsilon 1} C_{\epsilon 2} \bar{\rho} k \left(\frac{\partial \tilde{u}}{\partial r} \right)^2 - \frac{C_{\epsilon 2}}{C_D} \frac{\bar{\rho} \epsilon^2}{k}$$

convection

diffusion

production "source"

dissipation of ϵ "sink"